~~Maxvel~~

maxvell Em prediction = $c = \frac{1}{\sqrt{\varepsilon_0 \mu_0}}$

Expaimental evidance was in 1888 - Hertz

visible region [4.3×10^{14} Hz → 7.5×10^{14} Hz]

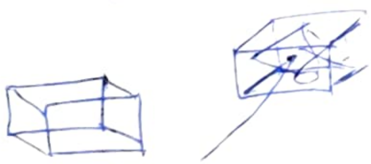
Radio wave ← | mico wave | IR | (visible) ~~VIBGYOR~~ ROYGBIV | UV | x-Ray | Gamary →

- Interference & difraction can be explained by wave theory
- young double slit experimentat light const of wave
- maxvell - theory

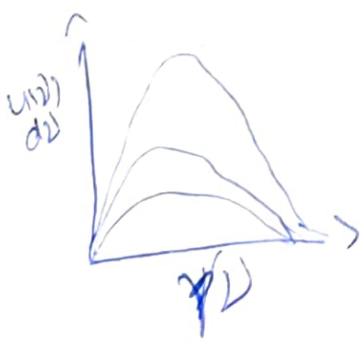
Black body Radiation

Radiation emited by bodys of mateu Are perfect emitor & ~~else~~ absorber of light (idealy)

idealy defind as a small cavity with pin hole.

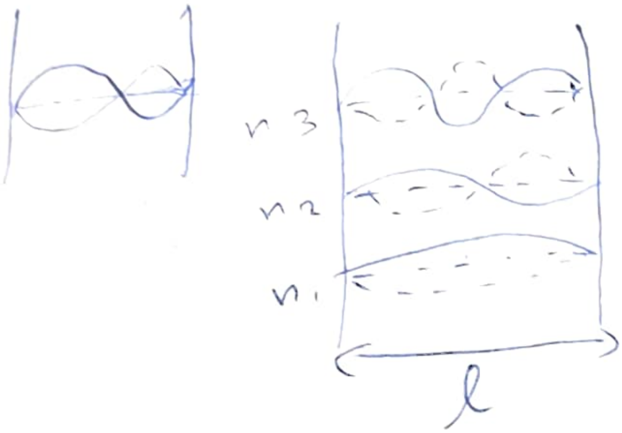


refled back and fort untill it get got absorbed, walls are constantly emitiz and absorbing radiation



Experimentaly

Inside the box Standing wave



$\frac{3\lambda}{2} = L$ =

$\lambda = L$ $\quad 2\frac{\lambda}{2} = L$

$\lambda = 2L$; $\frac{\lambda}{2} = L$

$L = n\frac{\lambda}{2}$

$\lambda = \frac{2L}{n}$

$\lambda = \frac{2\pi}{k}$ $= k = \frac{n\pi}{L}$

$\lambda = \frac{2\pi}{K}$, k = wave vector

$k = \frac{n\pi}{L}$ (Particl in 1D box)

$n = 1 \Rightarrow k = \frac{\pi}{L}$; $\lambda = \frac{2\pi}{\pi} L = 2L$

$n = 2 \Rightarrow k = \frac{2\pi}{2}$; $\lambda = \frac{2\pi}{2\pi} L = L$

Blackbody Spectrum In classical mechanic

Energy dencity of blackbody radiation

$u(\nu)d\nu = \bar{E}' G(\nu)d\nu$ — ①

(↑ dencity of standing wave
→ av. energ per standing wave

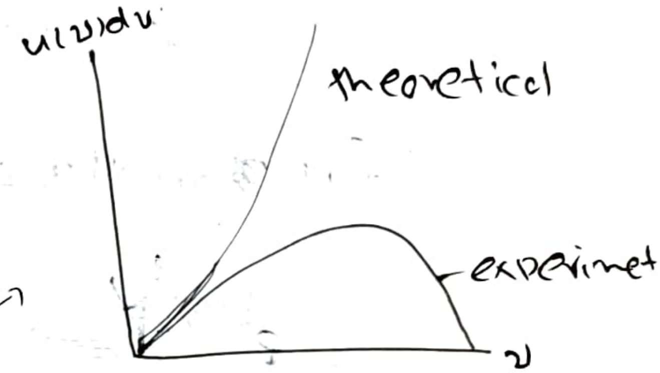
$G(\nu)d\nu$ = number of standing wave in unit Volue.

$= \frac{8\pi\nu^2}{c^3} d\nu$ → → derive this using sphecial shape

$\bar{\varepsilon}$ per degree of freedom
$\frac{1}{2}K_BT$, 3 dof freedom $\Rightarrow \frac{3}{2}K_BT$

Total KE+PE = K_BT

$\bar{\epsilon} = K_BT$ - (It is continues)



$u(\nu)\,d\nu = \frac{8\pi\nu^2}{c^3}\,d\nu\,KT$ → Ryleish Jeans formula

$\propto \nu^2$

Higher freqency. It fails (ultra violet catastrophic)

Planks modification

Planks - Radiation formula

change $\bar{\varepsilon}$ from KT to $\bar{\varepsilon} = \frac{h\nu}{e^{h\nu/KT} - 1}$, $h = 6.626 \times 10^{-34}$

$$u(\nu)d\nu = \bar{\varepsilon}\, G(\nu)d(\nu) = \frac{h\nu}{e^{h\nu/KT}-1} \cdot \frac{8\pi\nu^2}{c^3} d\nu$$

$$= \frac{8\pi h}{c^3} \frac{\nu^3 d\nu}{e^{h\nu/KT}-1}$$

At high freeqancy limit, $h\nu >> kT \Rightarrow e^{h\nu/KT} \to \infty$

$u(\nu)d\nu) \to 0$

At law freqeny, $h\nu << kT$

Tylor series expansion

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$$

for small $x \Rightarrow e^x = 1 + x$

$$\frac{1}{e^{h\nu/KT}-1} \approx \frac{1}{1+\frac{h\nu}{KT}-1} = \frac{KT}{h\nu}$$

$$u(\nu)d\nu = \frac{8\pi KT}{c^3} \nu^2 d\nu$$ — reileigh jeans formula

explanation

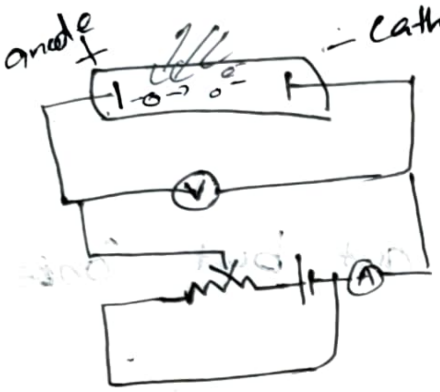
Oscilator of cavity walls Do not have Contineus destribution of energy but have discreate distribution. $\varepsilon_n = nh\nu$; $n = 0, 1, 2, 3, \ldots$

each discreate energy is Called quantum.

Energy transfer between atomic oscilator & Em waves are quantized. But Em wave is is contineus classical wave.

Photoelectric effect

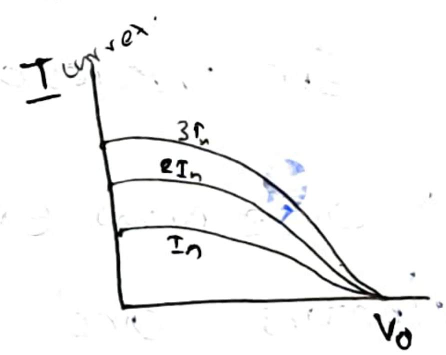
The energy of electron liberated by light depends up on the freqency of light.



Postulates

1. within notime $(10^{-9}s)$, photoelecton emits when light shines on the metal
(classically light is made of Em wave it should take some time to accumulate enough energy)

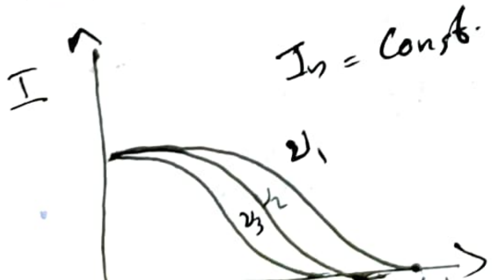
2. Bright light yields more photo electrons than a dim one at the same freqancy. but the electrons energy remain the same.



(retardent potential) maximum KE of e^- reaching at a cathode

(classicaly the more Intensity light the greater the energy of electrons

3. The higher the freqancy of light more the energy of photo electron have



$\nu_1 > \nu_2 > \nu_3$

at freqancy bellow a certain critical freqancy ν_0 no photo electon will emit.



linear increase in maximum photo electric energy

bellow perticlar freqency
No electrons are ~~alowded~~ exected.

Quntum theory of Light

1905, by Einstein

Energy ~~is~~ in the light is not spread out but Concentrat as small packets of light.

- Each photon of freqency ν have the energy $h\nu$ Same as that of planks Quntum Energy.

Em waves are quntized

1) Because now EM wave energy is Concentrated in photons and not spread out like wave frond There should be no delay. In the emmision of photoelectron.

2) All the photons of freqency ν have same energy. So changing the intencity of the light ~~beam~~ will change the no. of photoelectrons. but not their energys

3. Higher the freqeny ν greater the energy $h\nu$ so more energy the photo electrons have.

Meaning of Critical freqency (ν_0)

There must be minimum energy ϕ for an electron to escape from the perticular metal surface. This energy is called work function of the metel. $\phi = h\nu_0$.

According to Eientein photoelectric effect in a given metal should obay the equation. $h\nu = KE_{max} + \phi$

($h\nu$ → Photon energy; KE_{max} → maximum Photo electron energy; ϕ → work fn)

$$KE_{max} = h\nu - h\nu_0$$
$$= h(\nu - \nu_0)$$

what is light.
Both wave and particle

Wave nature → young's double slit experiment.
Particle nature → Photoelectric effect

Photoelectric effect → photon of light transfer energy to electron.

Inverse photoelectric effect
fast moving electron tranfer kinetic energy to metal eg (x-rays) to produce x-Rays

faster the original electron, the more penitrating the resulting x-ray

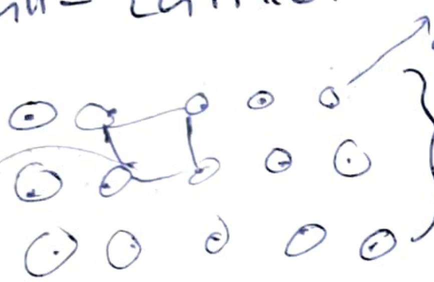
Greater the number of electron, greater the intencity of x-ray.

X-Ray-Difraction

Scattering of x-ray beam from crystal plane

ie) braggs plane

Crystal = Lattice + Basis

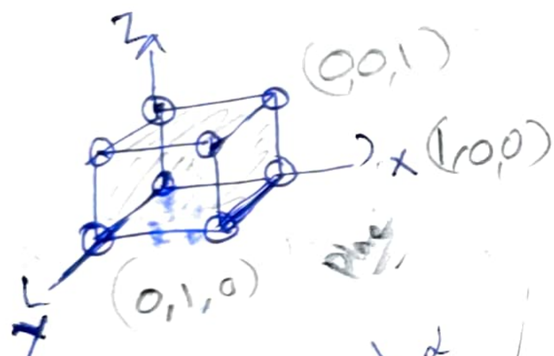


lattice — like Periodic arragements of Points

→ Periodic arragements of atoms.

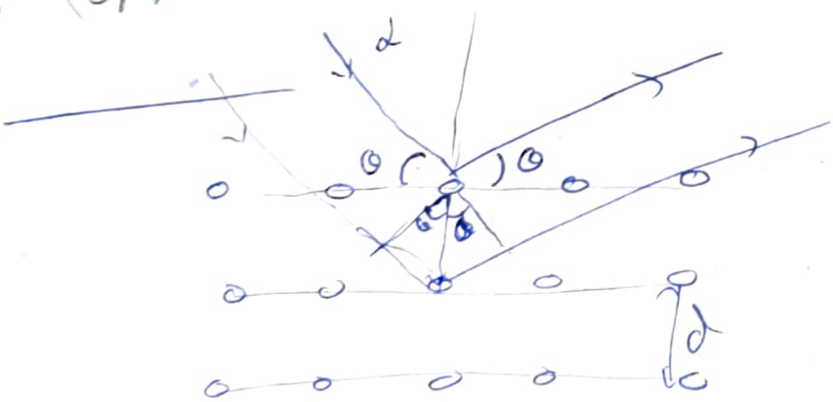
→ Unit cell ⇒ Smallest repeating unit in a Crystal

(∞ ∞ 1) $\left(\frac{1}{\infty}, \frac{1}{\infty}, \frac{1}{1}\right)$



Path difference = $n\lambda$

~~$n\lambda = 2d\sin\theta$~~



for constructive interfearence.

$n\lambda$ = Path diff. $= 2d\sin\theta$.

$n\lambda = 2d\sin\theta$, braggs diffraction condition.

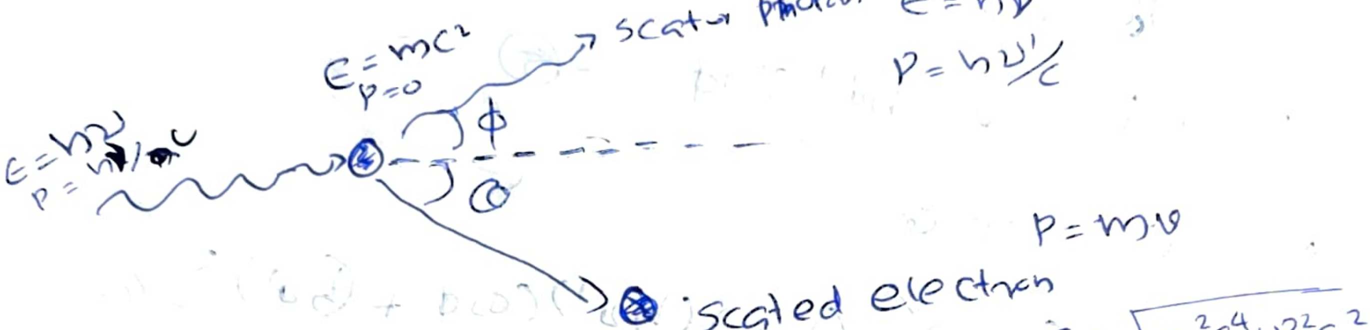
$n = 1, 2, 3, \ldots$

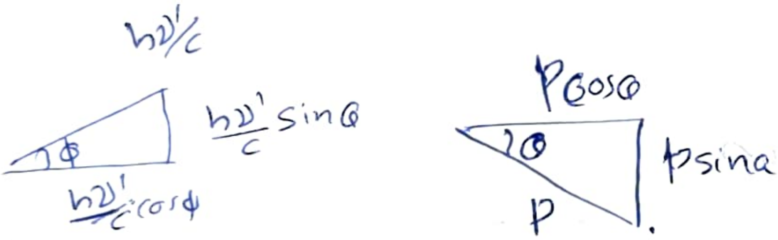
Compton effect

further establish photon model

change in the wave length. of photon Scattered from Particle (electron at rest).

$$\lambda' - \lambda = \frac{h}{m_0 c}(1 - \cos\phi)$$





Totel Energy & momentum should remain conserved

Conservation of energy.

Loss of photon energy = gain in the electron KE ~~energy~~.

~~$h(\nu - h\nu') = KE$~~

$$h\nu - h\nu' = KE \quad (1)$$

Conservation of momentum ⇒ T

initial momentum = final momentum

$$\frac{h\nu}{c} + 0 = \frac{h\nu'}{c}\cos\phi + p\cos\theta \quad (2)$$ ||el componi

$$0 + 0 = \frac{h\nu'}{c}\sin\phi - p\sin\theta \quad (3)$$

$$(2) \Rightarrow pc\cos\theta = h\nu - h\nu'\cos\phi \quad (4)$$

$$(3) \Rightarrow pc\sin\theta = h\nu'\sin\phi \quad (5)$$

] sqrin & add

to eliminate θ

$$p^2c^2 = (h\nu)^2 - 2(h\nu)(h\nu')\cos\phi + (h\nu')^2 \quad (6)$$

Energy Conservation

$$(h\nu + mc^2) = h\nu' + \sqrt{m^2c^4 + p^2c^2}$$

$$m^2c^4 + p^2c^2 = [h\nu - h\nu' + mc^2]^2$$

$$p^2c^2 = (h\nu - h\nu')^2 + m^2c^4 + 2(h\nu - h\nu')mc^2 - m^2c^4$$

$$p^2c^2 = h\nu^2 - 2h\nu h\nu' + (h\nu')^2 + 2mc^2(h\nu - h\nu') \quad (7)$$

(6) in (7) ⇒ we have

$$(h\nu)^2 - 2h\nu\, h\nu' \cos\phi + (h\nu')^2 = (h\nu)^2 - 2h\nu\, h\nu' + (h\nu')^2 + 2mc^2 h(\nu -$$

$$\Rightarrow 2mc^2(h\nu - h\nu') = 2h\nu\, h\nu'.(1-\cos\phi) \quad - (8)$$

$$2mc^2 h/c\left(\frac{\nu}{c} - \frac{\nu'}{c}\right) = 2h^2 c^2\left(\frac{\nu}{c}\frac{\nu'}{c}\right)(1-\cos\phi)$$

$$\frac{mc}{h}\left(\frac{\nu}{c} - \frac{\nu'}{c}\right) - \frac{\nu\nu'}{c^2}(1-\cos\phi) \qquad \frac{\nu}{c} = \frac{1}{\lambda}$$

$$\frac{mc}{h}\left(\frac{1}{\lambda} - \frac{1}{\lambda'}\right) = \frac{1-\cos\phi}{\lambda\lambda'}$$

$$\frac{mc}{h}\left(\frac{\lambda' - \lambda}{\lambda\lambda'}\right) = \frac{1-\cos\phi}{\lambda\lambda'} \Rightarrow \boxed{\lambda' - \lambda = \frac{h}{m_0 c}(1-\cos\phi)}$$

Compton wavelength (λ_c)

$$\lambda' - \lambda = \lambda_c(1-\cos\phi)$$

Greatest lamda (λ) change ~~as cos~~ Corresponds to $\phi = 180$

$$\lambda' - \lambda = 2\lambda_c$$

Pairproduction

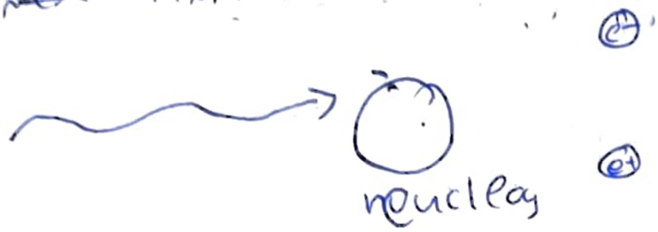
Energy into matter (mass)

photoelectic effect → all energ given to electron

Partical Energy is given → compton effect.

photon materialise into electron & and positron → Pair Production

Electro magnetic energy get Converted in ~~m~~ matter



Proton & positron

Same charge +1   +1

have mass of e-

3 quarks (2UP 1down)

mass ≃ 1800x more than Positron

Pair production obays charge Conservation.

total energy & linear momentum are Conserved

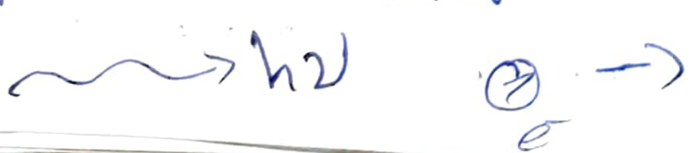
rest mas energy of e^- = 0.51MeV

e^+ = 0.51 mev

Pair production requires photon energy at atleast 1.02 Mev   ~ 1mev = 10^6 eV   (γ-rays)

cosmic rays & emmision from the radio active neucli

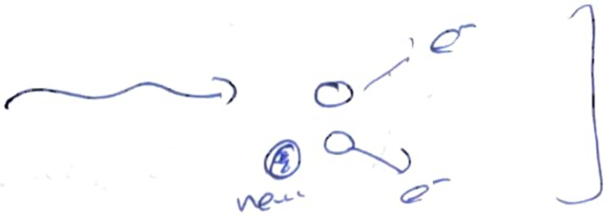
photoelectric effect.



Compton Scatering



low energy Process

Pairproduction 

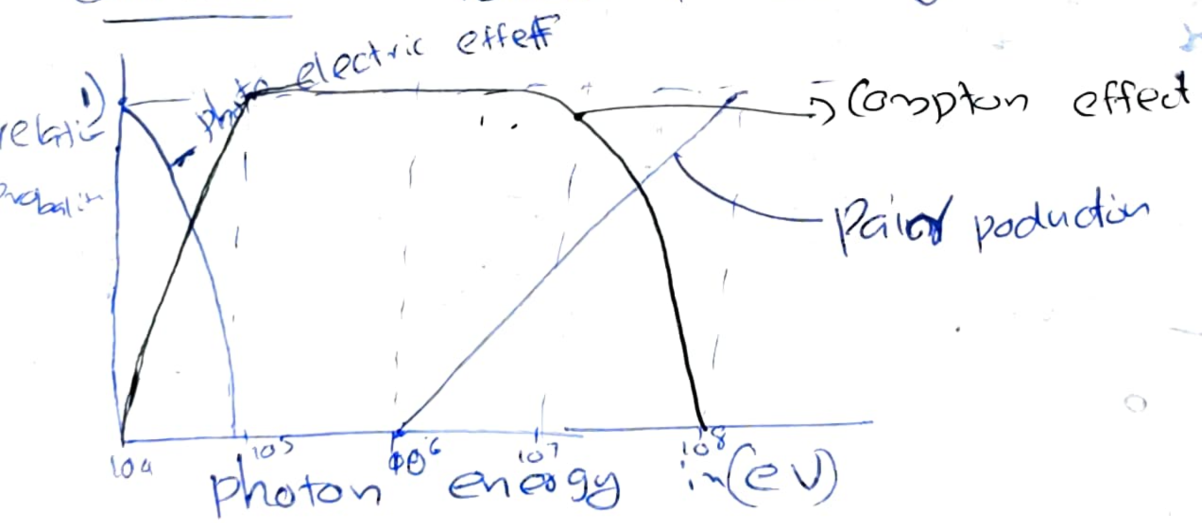
high energy.

In these phenaminon photon energy ranges from $10^4 eV$ to $10^8 eV$

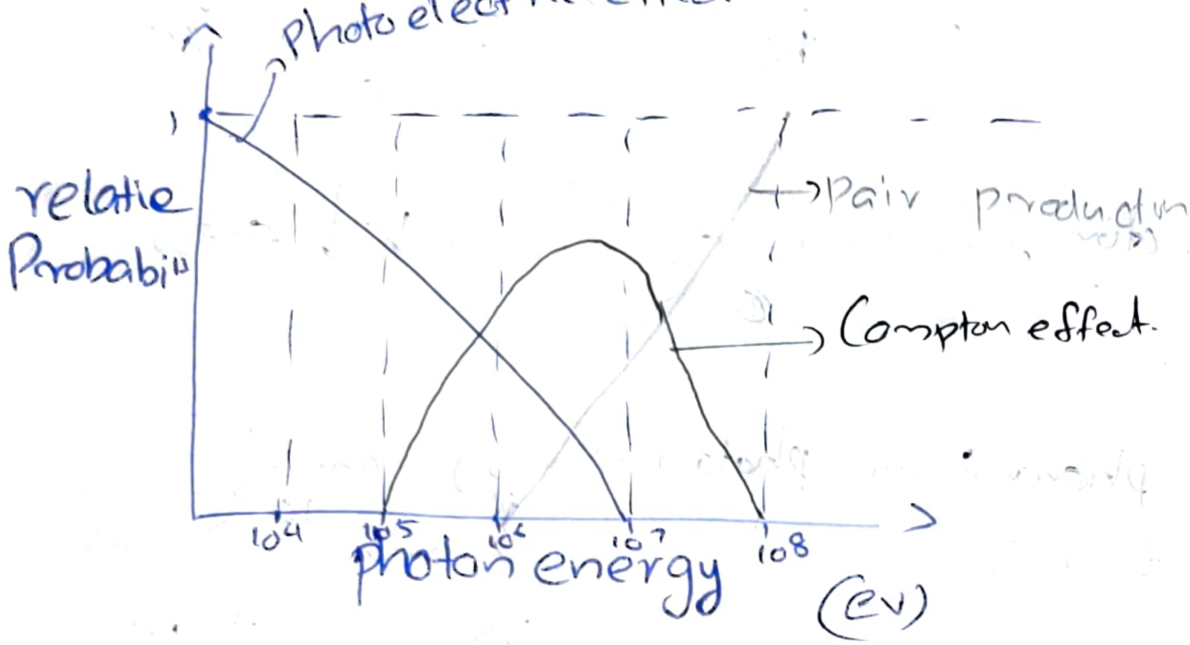
γ –	$10^5 - 10^8$
X-ray	$= 10^3 - 10^5$
Uv –	$= 10^1 - 10^3 eV$
visible	$1 - 10 eV$
IR	$10^{-3} - 1 eV$
micro	$10^{-5} - 10^{-3} eV$
radio	$10^{-11} - 10^{-5} eV$

Carbon

relative probability.



Lead (Pb)



Photons & Gravity

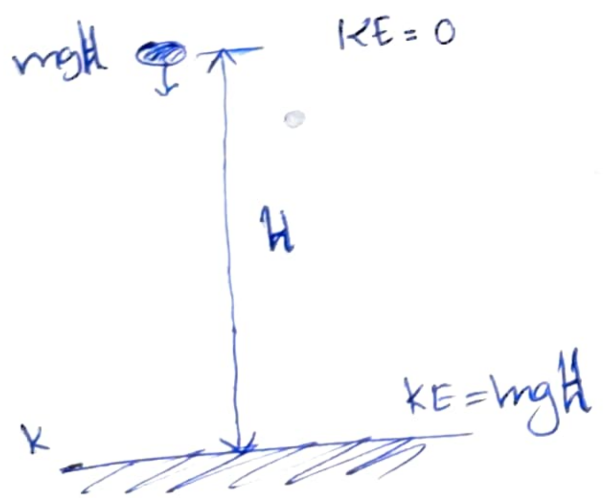
nearly (zero rest mass). they behave like as they ~~Bet~~ have Gravitational mass

$mc^2 = mvc$

$E = pc$

Photon mass : $m = \frac{p}{v} = \frac{h\nu}{c^2}$ —(1) $p = \frac{E}{c} = \frac{h\nu}{c}$

{ $E = h\nu$ }



$E = h\nu + mgH$

$= h\nu + \left(\frac{h\nu}{c^2}\right)gH = h\nu'$

$$h\nu' = h\nu + \frac{h\nu}{c^2} gH$$

$$\boxed{h\nu' = h\nu\left(1 + \frac{gH}{c^2}\right)}$$

B

De-Broglie wave

1924 - moving objects have wave aswell as particle nature.

Everymoving objects have wave assosiated with it. is called matter wave.

$$\boxed{\lambda = \frac{h}{p}}$$ → General relation that can be applied to photons as well as material particle.

momentum of particle with mass m & veloci

$p = \gamma m_0 v$ ~~v~~ ~~...~~ $\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}$

matter wave/De-Broglie wave?

water wave → Quantity that ~~varry~~ varry periodicaly (Hight of the whater Surface)

Sound wave → Pressure varries

Light wave → electric & magtic field vector.

matter wave → $\psi(x,y,z)$ - no physical significance

ψ^2 = Probability dencity

waves of probability

- The value of a wavefunction associated with moving body at perticular point (x,y,z) in space at time t is related with the probability of finding that body at time t

ψ → No direct physical significance and experimentaly not observable.

ψ^2 → Probability dencity which is experimently observable.

Description of debroglie wave.

Debroglie wave velocity. $V_p = \nu\lambda$

$\lambda = \frac{h}{\gamma m v}$

velocity v observe

$E = \gamma m c^2$

$\nu = \frac{\gamma m c^2}{h}$

$V_p = \frac{\gamma m c^2}{h}\left(\frac{h}{\gamma m v}\right) = \frac{c^2}{v}$

$V_p = \nu\lambda$ → $E = h\nu = \gamma m_0 c^2$

$\nu = \frac{\gamma m_0 c^2}{h}$

$V_p = \frac{c^2}{v}$

$\lambda = \frac{h}{\gamma p} = \frac{h}{\gamma m_0 v}$

refer ⇒

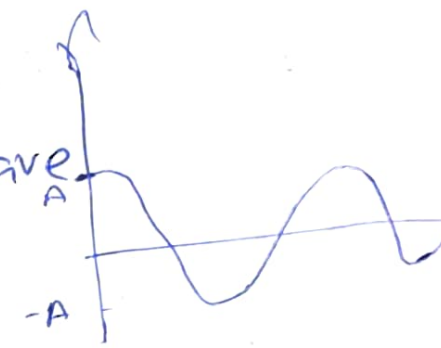
⇒ $V_p = \frac{c^2}{v}$ → velocity of moving body that must be less than velocity of light (c)

⇒ $V_p > c$ ⇒ debroglie waves move faster than light. # not possible.

This is not physically correct.

Phase and group velocities

Representation of De-broglie wave



$y = A\cos(\omega t - kx)$ → ① wave vector

↑ amplitude, ↖ anguarf freqeny

- A wave representation of a moving body correspond to wave packet or wave group.

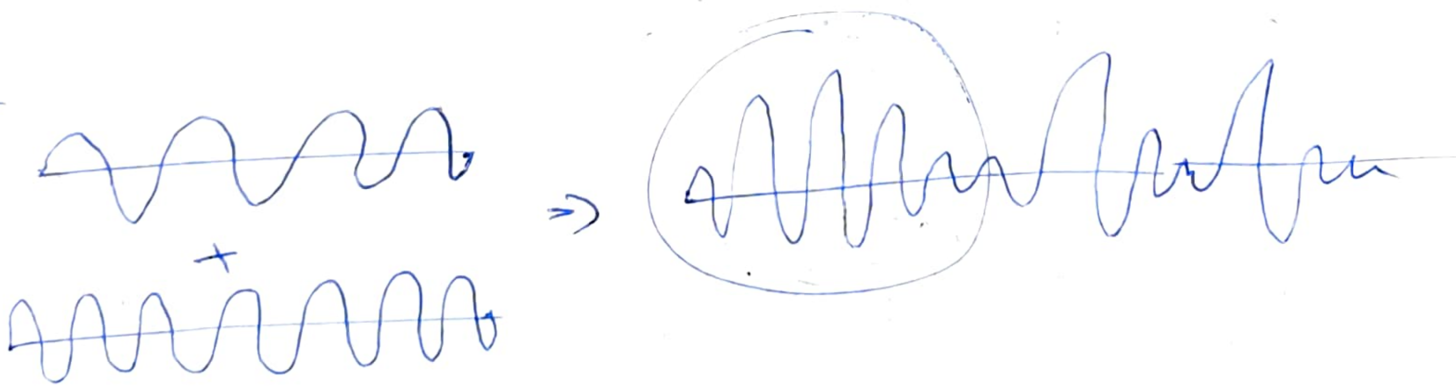


these are the superposition of individual wave of wavelengths whoe interferenie with one another wave paket

\ wavepacket

⇒

wave groups



phase velocity $= V_p = \frac{\omega}{K}$ — ①

Group velocity $= V_g = \frac{d\omega}{dK}$ — ②

$$\omega = 2\pi\nu = \frac{2\pi\gamma mc^2}{h} = \frac{2\pi mc^2}{h\sqrt{1-v^2/c^2}} \quad — ③$$

$$K = \frac{2\pi}{\lambda} = \frac{2\pi\gamma mv}{h} = \frac{2\pi mv}{h\sqrt{1-v^2/c^2}} \quad — ④$$

$$V_g = \frac{d\omega}{dK} = \frac{d\omega/dv}{dK/dv} \quad , \quad \cancel{\frac{d\omega}{dv}} = \cancel{\frac{2\pi}{m}}$$

$$\frac{d\omega}{dv} = \frac{2\pi mc^2}{h}\left[-\frac{1}{1-v^2/c^2}\frac{d}{dv}\left(1-v^2/c^2\right)^{1/2}\right]$$

$$= \frac{2\pi mc^2}{h}\left[-\frac{1}{(1-v^2/c^2)}\cdot\frac{1}{2}\left(1-\frac{v^2}{c^2}\right)^{-1/2}\cdot\left(\frac{-2v}{c^2}\right)\right]$$

$$\frac{d\omega}{dv} = \frac{2\pi mv}{h}\left[\frac{1}{(1-v^2/c^2)^{3/2}}\right] \quad — ⑥$$

∴ ~~similarly~~ $\frac{dK}{dv} =$

~~Similarly~~ = $\frac{d\omega}{dv} = \frac{2\pi m_0 v}{h\left[1-v^2/c^2\right]^{3/2}}$

Similarly - $= \frac{dk}{dv} = \frac{2\pi m_0}{h\left(1-\frac{v^2}{c^2}\right)^{3/2}}$

$= \frac{2\pi m_0}{h} \times \frac{\sqrt{1-v^2/c^2} - \frac{v^2}{\cancel{2}\sqrt{1-v^2/c^2}}}{(1-v^2/c^2)}$ $= \frac{\left(1-\frac{v^2}{c^2}\right) - v^2}{(1-v^2/c^2)^{3/2}}$

$= \frac{1}{(1-v^2/c^2)^{1/2}} - \frac{v^2}{(1-v^2/c^2)^{3/2}} = \frac{1}{(1-v^2/c^2)}\left(\frac{\left(1-\frac{v^2}{c^2}\right) - v^2}{(1-v^2/c^2)}\right)$

$\frac{dk}{dv} = \frac{2\pi m}{h\left(1-\frac{v^2}{c^2}\right)}$ - (7)

Put (6) & (7) in eq^n (5)

$\Rightarrow$ (5) $\Rightarrow$ $V_g = v$ (velocity of move body)

Debroglie wave packets associated with the moving body travels with the same velocity of the body

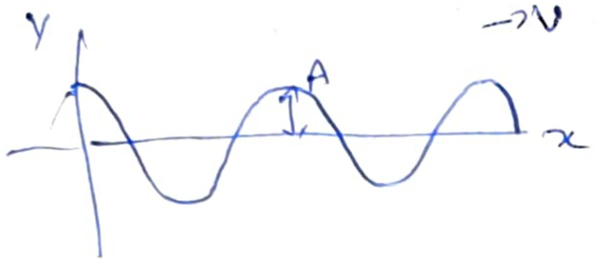
De-broglie wave velocity doesn't have no physical significants $\left(V_p = \frac{\omega}{k} = \frac{c^2}{v}\right)$

Because motion of the body depend on V_g

Shrödinger wave equation

There is no derivation.

Assume that any particle is freely moving in x direction ;



$y = A\cos\omega t$ — standing wave —①

$y = A\cos\omega\left(t - \frac{x}{v}\right)$ — Traveling wave. —②

$\psi = A\cos\omega\left(t - \frac{x}{v}\right) - iA\sin\omega\left(t - \frac{x}{v}\right)$ —③

$\psi = Ae^{-i\omega\left(t - \frac{x}{v}\right)}$ —④ spherical wave travels in x direct.

$\omega = 2\pi\nu$

$v = \nu\lambda$

$\psi = Ae^{-2\pi i\left(\nu t - \frac{x}{\lambda}\right)}$ —⑤

$E = h\nu$

$E = \hbar 2\pi\nu$

$\psi = Ae^{-\left(\frac{i}{\hbar}\right)[Et - px]}$ —⑥

$\lambda = \frac{h}{p} = \frac{2\pi\hbar}{p}$

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{-p^2}{\hbar^2} \psi$$

$$p^2 \psi = -\hbar^2 \frac{\partial^2 \psi}{\partial x^2} \quad — (7)$$

$$\frac{\partial \psi}{\partial t} = \frac{iE}{\hbar} \psi \quad — (8)$$

$$E\psi = \frac{-\hbar}{i} \frac{\partial \psi}{\partial t}$$

Totel Energy = KE + PE

$$E = \frac{p^2}{2m} + U(x,t) \quad — (9)$$

$$E\psi = \frac{p^2}{2m}\psi + U\psi \quad — (10)$$

Time depended Shrödinger eq^n

using (7) & (8) in (10)

$$(10) \Rightarrow \boxed{i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U\psi} \quad — (11)$$

Shrödinger wave eq^n In 1D

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \psi + U\psi$$

Shrödinger wave eq^n Cannot derive from other principle of physic. It is it's self a Principle.

Time indipendend Shrödinger eqn

if PE & F ...

$U = U(x)$

$\Psi = A e^{-(i/\hbar)(Et - px)}$ — (*)

$\Psi = A e^{-i\left(\frac{E}{\hbar}\right)t} \cdot e^{i(p/\hbar)x}$ — (*) ← time indipendent

$\Psi = \psi_0 e^{-i\left(\frac{E}{\hbar}\right)t}$ — (1)

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U\psi \quad \text{— (2)}$$

Put (1) in (2) ⇒

independent

(2) ⇒ $E\psi e^{-i\left(\frac{E}{\hbar}\right)t} = \frac{-\hbar^2}{2m} e^{-\left(\frac{iE}{\hbar}\right)t} \cdot \frac{\partial^2 \psi}{\partial x^2} + U\psi e^{-\left(\frac{iE}{\hbar}\right)t}$

$$\Rightarrow \frac{-\hbar^2}{2m} \frac{\partial \psi}{\partial x^2} + (E - U)\psi = 0$$

$$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - U)\psi = 0$$

Hamitonian Operator ($\hat{H}$) = $\hat{KE} + \hat{U}$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U$$

$\psi = Ae^{-i/\hbar(Et - px)}$

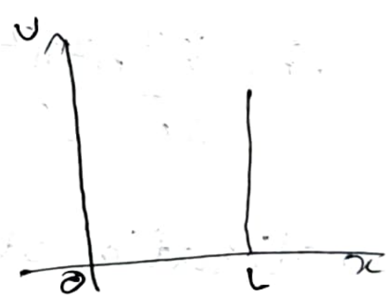
$\frac{\partial\psi}{\partial x} = \psi \frac{i}{\hbar} p$

$p = \frac{\hbar}{i}\frac{\partial}{\partial x}$

Shrodingen eqn = $\hat{H}\psi = E\psi$

Quntity	Operator
Position, x	$\hat{x}$
p	$-i\hbar\frac{\partial}{\partial x}$
KE	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
total energy	$i\hbar\frac{\partial}{\partial t}$
PE	$\hat{U}$

Particle In a box



Shrodinger eqn can be written as

$U = \infty$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}E\psi = 0 \quad -(1)$$

$U = 0$ inside the box

$$\Rightarrow \frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad -(2), \quad k^2 = \frac{2mE}{\hbar^2} \therefore k = \frac{\sqrt{2mE}}{\hbar}$$

Boundary Conditions – $\psi = 0$; $x \le 0$, $x \ge L$

Solution of these kind of DE in Sin & Cos

(2) $\Rightarrow \psi = A\sin kx + B\cos kx$ — (3)

At $x = 0$, $\psi = 0$

(3) $\Rightarrow 0 = 0 + B\cos k0$

$B = 0$

At $x = L$, $\psi = 0$

(3) $\Rightarrow L = A\sin kL + B\cos kL$

$L = A\sin kL$

$A \neq 0 \Rightarrow \sin kL = 0$

$kL = n\pi$

$k = \frac{n\pi}{L}$, $n = 1, 2, 3 \ldots$

(3) $\Rightarrow \psi = A\sin kx$ — (4)

(4) $\Rightarrow$ $\boxed{\psi_n = A\sin\frac{n\pi}{L}x}$ — (5), $n = 1, 2, 3, 4 \ldots$

$\sqrt{2mE} = \hbar k$, $k = \frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{L}$

$E = \frac{\hbar^2 k^2}{2m}$ or

$\Rightarrow E_n = \frac{\hbar^2 n^2 \pi^2}{2m L^2}$ — (6)

Normalization of the wave function ψ

$$\boxed{\int_{-\infty}^{\infty} \psi_n^* \psi_n \, dx = 1}$$

Probability = 1
— Normalization Condition

$$\int_0^L A^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

$\sin^2\theta = \frac{1 - \cos 2\theta}{2}$

$$\Rightarrow A^2 \int_0 \frac{1}{2}\left[1 - \cos\left(\frac{2\pi n x}{L}\right)\right] dx = 1$$

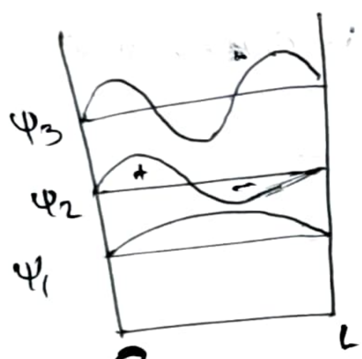
$$\frac{A}{2}\left[\int_0^L dx - \int_0^L \cos\left(\frac{2n\pi x}{L}\right) dx\right] = 1$$

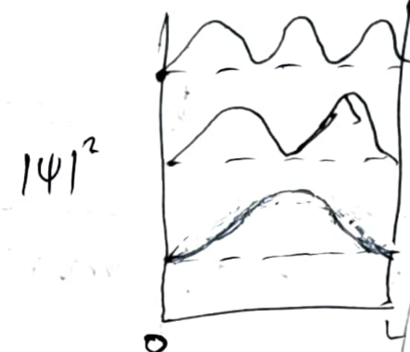
$= 0$

$$\frac{A^2}{2}[L] = 1$$

$$A = \sqrt{\frac{2}{L}}$$, Amplitude

(5) $\Rightarrow \psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x$





Momentum of the particle Confined inside one (1D box)

~~box~~ $\psi = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x$ — (1) $\langle \hat{A} \rangle \frac{\int_{-\infty}^{\infty} \hat{A} |\psi|^2 dx}{\int_{-\infty}^{\infty} |\psi|^2 dx}$ — Normali[illegible]

expectation Value

any operator $\hat{A}$, $\langle \hat{A} \rangle = \int_{-\infty}^{\infty} \psi^* \hat{A} \psi dx$ — Normaliz[illegible]

$$\langle \hat{p} \rangle = \int_{-\infty}^{\infty} \psi^* \hat{p} \psi dx = \int_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \psi dx$$

$$= -i\hbar \int_0^L \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x \sqrt{\frac{2}{L}} \left(\frac{n\pi}{L}\right) \cos\left(\frac{n\pi}{L}\right) x \, dx$$

Expetation Value

like MI

$$\langle x \rangle = \frac{\sum N_i x}{\sum x_i}$$

$N_i \Rightarrow$ how [illegible]

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} |\psi|^2 [illegible]}{\int_{-\infty}^{\infty} |\psi|^2 dx}$$

Prodect[illegible]

$|\psi|^2 = \psi^* \psi$

$$= i\hbar\left(\frac{2}{L}\right)\left(\frac{n\pi}{L}\right)\int_0^L \sin\left(\frac{n\pi}{L}\right)x \cdot \cos\left(\frac{n\pi}{L}\right)x\,dx \quad -(2)$$

$$\int \sin ax \cos ax\,dx = \frac{1}{2a}\sin^2 ax$$

$$(2) \Rightarrow \langle\hat{p}\rangle = -i\hbar\left(\frac{2}{L}\right)\left(\frac{n\pi}{L}\right)\frac{1 \cdot L}{2n\pi}\left[\sin^2\left(x\frac{n\pi}{L}\right)\right]_0^L$$

$$\langle p\rangle = 0$$

At first instant it seems very strange

$$E = \frac{p^2}{2m}$$ because it is avg value

$$p_n = \pm\sqrt{2mE_n} = \pm\sqrt{\frac{2m \cdot n^2\pi^2\hbar^2}{2mL^2}}$$

$$p_n = \pm\sqrt{\frac{n^2\pi^2\hbar^2}{L^2}} = \pm\frac{n\pi\hbar}{L}$$

Since particle is moving back and forth. So average momentum for any value of n is given by

$$p_{av} = \frac{\left(\frac{n\pi\hbar}{L} + \frac{-n\pi\hbar}{L}\right)}{2} = 0$$

$\lambda = \frac{2\pi}{K}$, $K = \frac{n\pi}{L}$

$\varepsilon_0 = 8.85 \times 10^{-12}$ F/m

$\mu = 4\pi \times 10^{-7}$

$K = 1.38 \times 10^{-23}$ J/K

$h = 6.626 \times 10^{-34}$ J.s

$m_e = 9.1 \times 10^{-31}$ kg

$eV = 1.6 \times 10^{-19}$ J

$m_e c^2 = 0.51$ MeV

Black body

$U(\nu)d(\nu) = \bar{\varepsilon}\, G(\nu)\, d(\nu)$

energy densit

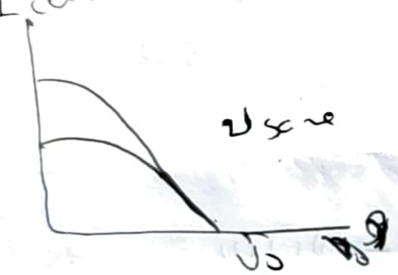
, $\bar{\varepsilon} = K_B T$ $G(\nu) = \frac{8\pi\nu^2}{c^3} d\nu$

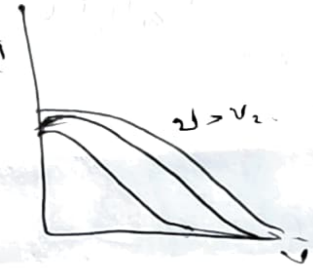
$U(\nu)d(\nu) = \frac{8\pi\nu^2}{c^3} K_B T\, d\nu$, Reyleigh-Jeans

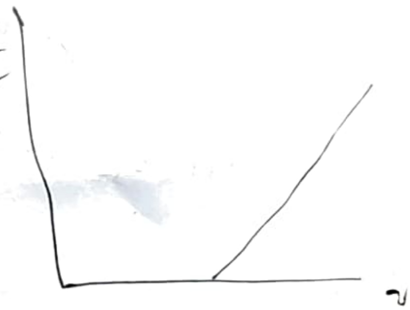
Planks modification, $\bar{\varepsilon} = \frac{h\nu}{e^{h\nu/KT} - 1}$

$E_n = nh\nu$

Photo electric







$KE_{max} = h\nu - h\nu_0$ work function

$n\lambda = 2d\sin\theta$, Braggs for constructive interference.

$\lambda' - \lambda = \frac{h}{m_0 c}(1 - \cos\phi)$ Compton effect , $\lambda_c = 2.42$ pm

$E^2 = p^2c^2 + m_0^2c^4$ If $v = 0 \Rightarrow E = m_0 c^2$

$p = \frac{h\nu}{c} = \frac{h}{\lambda} \Rightarrow h\nu = pc$

Pair production

in presents of heavi nucleon.

$m_e c^2 = 0.51$ MeV

mgh or $-\frac{GM}{r}$

Photon & Gravity

$m = \frac{p}{v} = \frac{h\nu}{c^2}$ $h\nu = m_0 c^2$



$h\nu' = h\nu + mgH \Rightarrow h\nu\left(1 + \frac{gH}{c^2}\right)$

$\lambda = \frac{h}{p}$, debroglie wave, / $p = \gamma m_0 v$, $\gamma = \frac{1}{\sqrt{1-\frac{c^2}{v^2}}}$

$V_p = \nu\lambda$, $\nu = \frac{\gamma m_0 c^2}{h}$, $\lambda = \frac{h}{\gamma m_0 v}$

$= \frac{c^2}{v}$

$\omega = 2\pi\nu$, $K = \frac{2\pi}{\lambda}$

$V_p = \frac{\omega}{K}$,

standing wave

$V_g = \frac{d\omega}{dk}$, $\frac{d\omega}{dv} \times \frac{dv}{dk}$ $\Rightarrow$ $V_g = v$

$y = A\cos\omega t$ – travelling wave.

$y = A\cos(\omega t - x/v)$

$pc = \frac{hc}{\lambda}$ | $mc^2 = m_0c^2 + KE$

$\psi = Ae^{-i\omega(t - x/v)}$, $\omega = 2\pi\nu$

$v = \nu\lambda$

$|\psi|^2 = \psi^*\psi$, $\psi = Ae^{-(i/\hbar)(Et - px)}$, $\lambda = \frac{\hbar 2\pi}{p}$

$E = 2\pi\hbar\nu$

$\int_{-\infty}^{\infty} |\psi|^2 dV = 1$, Normalization

$\nabla^2 y = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}$

$E = \frac{p^2}{2m} + U(x,t)$ $\times\psi$ $\Rightarrow$ $i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m}\nabla^2\psi + U\psi$ – time dependent Shro-

$\psi = \psi e^{-\frac{iEt}{\hbar}}$

$\Rightarrow \nabla^2\psi + \frac{2m}{\hbar^2}(E-U)\psi = 0$

$\hat{p} = -i\hbar\frac{\partial}{\partial x}$

$KE = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

$\frac{\partial^2\psi}{\partial x^2} + k^2\psi = 0$

$E = i\hbar\frac{\partial}{\partial t}$

Particle inside a box

$K = \frac{\sqrt{2mE}}{\hbar}$ $\Rightarrow E = \frac{\hbar^2 n^2\pi^2}{2mL^2}$

$\Rightarrow \psi = A\sin kx + B\cos kx$

$K = \frac{n\pi}{L}$

$\Rightarrow \psi_n = A\sin\frac{n\pi}{L}x$, $n = 1, 2, \cdots$

$\langle\hat{p}\rangle = 0$

normalized $\Rightarrow$ $\psi_n = \sqrt{\frac{2}{L}}\sin\frac{n\pi}{L}x$

$p = \sqrt{2mE} = \pm\frac{n\pi\hbar}{L}$

$\langle x \rangle = \frac{\sum N_i x_i}{\sum x_i}$ here $N_i = P_i$ like cm.

$\langle x \rangle = \frac{\int_{-\infty}^{\infty} |\psi|^2 x \, dx}{\int_{-\infty}^{\infty} |\psi|^2 dx}$ $\quad \langle \vec{p} \rangle = \frac{\int_{-\infty}^{\infty} \psi^* \vec{p} \psi \, dx}{\int_{-\infty}^{\infty} |\psi|^2 dx = 1 \text{ normalized}}$

Hilbert Space

$(\psi, \phi) = (\phi, \psi)^*$, $(\psi, \phi) = \psi^* \phi \Rightarrow (\psi, \phi) \neq (\phi, \psi)$

$(\phi, a\psi, b\psi_2) = a(\phi, \psi) + b(\phi, \psi_2)$ → linear

$(a\phi_1 + b\phi_2, \psi) = a^* (\phi, \psi) + b^* (\phi_2 \psi)$ = antinear

$(\psi, \psi) = |\psi|^2 \Rightarrow \psi^* \psi$

Dirac notation

$(\phi, \psi) \Rightarrow \langle \phi | \psi \rangle$ $\quad | \quad \langle \phi | \psi \rangle^* = \langle \psi | \phi \rangle^*$

$\Rightarrow \int \phi^*(r,t) \, \psi(r,t) \, d^3r$

$|a\psi\rangle = a|\psi\rangle$; $\langle a\psi| = a^* \langle \psi|$

Schartz inequality

$\langle \psi | \phi \rangle^2 \leq \langle \psi | \psi \rangle \langle \phi | \phi \rangle \Rightarrow |\vec{A} \cdot \vec{B}|^2 \leq |\vec{A}|^2 |\vec{B}|^2$

Triagle ensechr

$\sqrt{\langle \psi + \phi | \psi + \phi \rangle} \leq \sqrt{\langle \psi | \psi \rangle} + \sqrt{\langle \phi | \phi \rangle} \Rightarrow |\vec{A} + \vec{B}| \leq |\vec{A}| + |\vec{B}|$

$\langle \psi | \phi \rangle = 0$, orthogonal , $\langle \psi | \phi \rangle = 1 \Rightarrow$ orthonormal.

$\langle \psi | \psi \rangle = 0 =$

$|\psi\rangle|\phi\rangle$, $\langle \phi| \langle \phi|$, forbiden

Mathamatical ~~formulation~~ Tools of QM

Formulation of QM
→ shrödinger wave mechanics
→ Heisenberg matrix ~~mathan~~ machanics.

→ It deals with operators which are linear and wavefunction that belongs to Hilberts Space.

Linear Vector space

It Consists of 2 sets of elements and two algebric rules.

- set of vects ψ, ϕ, χ
- Set of scalar $a, b, c,$

rules of vector addition
" scalar multiplication

Addition rule:-

1. If ψ, ϕ are vector then $\psi + \phi$ is also a closed vector of same space.

2. Commutativity: $\psi + \phi = \phi + \psi$

3. Associativity: $(\psi + \phi) + \chi = \psi + (\phi + \chi)$

4.) Existance of zero or neutral vector such that
$$\psi + 0 = 0 + \psi = \psi$$

5.) Existence of symmetric or inverse vector

$$\psi + (-\psi) = (-\psi) + \psi = 0$$

Mutiplicatin Rules

also closed under mutiplication

1.) mutiplication of vector by scalar give, anther vector. If ψ & ϕ are two vector of the space, any linear Combination of $a\psi + b\phi$ is also a vector of that space (a, b, are scalar)

$$a\psi = \psi a \leftarrow \text{commutative}$$

2. Distribeutivity

$$a(\psi + \phi) = a\psi + a\phi$$

$$(a+b)\psi = a\psi + b\psi$$

3. Associativiy

$$a(b\psi) = (ab)\psi$$

4) for each element ψ there must exis a unitary scalar and zero '0' such that

$$I\psi = \psi I = \psi$$

$$0\psi = \psi 0 = 0$$

Hilbert space (H)

Consists of set of vector $\psi, \phi, \chi, \ldots$, and set of scalars such as $a, b, c \ldots$ which satisfy following properties

1. H is linear space, all the properties of linear vector space is obay by H

2. H has defind scalar product that is strickly +ve

we have scalar product of an element ψ with another element ϕ which is in general a complex number denoted by (ψ, ϕ)

$(\psi, \phi) = \psi^* \phi$

$(\psi, \phi) \neq (\phi$

$$(\psi, \phi) = (\phi, \psi)^*$$

$$(\phi, a\psi_1 + b\psi_2) = a(\phi, \psi_1) + b(\phi, \psi_2)$$

$$(a\phi_1 + b\phi_2, \psi) = a^*(\phi_1, \psi) + b^*(\phi_2, \psi)$$

$$(\psi, \psi) = |\psi|^2 \geq 0$$

$*$ Complex

Note :- In scalar product, (ϕ, ψ), second vector ψ belongs to hilberts space H, while ϕ first vector ϕ belongs to dualspace. (H_d) ↳ also hilbert space

But Commutate property not obayed
i.e. $(\phi, \psi) \neq (\psi, \phi)$, (Scalar Product is not commutated.)

3) H is seperable,
There exist a cauchy sequence $\psi_n \in H$ $(n = 1, 2, 2,)$ such that for every ψ of H there is at least one ψ_n of the sequence for which $|\psi - \psi_n| < \epsilon$, $\epsilon > 0$

4) H is Complete :- Every Cauchy sequence $\psi_n \in H$ converges to an element of Hilbert space H
ie for any ψ_n, $\lim_{n,m \to \infty} |\psi_n - \psi_m| = 0$

$$\lim_{n \to \infty} |\psi - \psi_n| = 0$$

Wave function live in Hilbert Space.

Dirac Notation

State vectors,

~~elements of~~

The physical state of a system is represented in QM by elements of Hilberts Space. are called State vectors.

kets – Elements of Hilberts ~~ba~~ space. $|\rangle$

$\psi \rightarrow |\psi\rangle$

Bras → Elements of dual space. $\langle|$

$\langle\phi|$

Dirac Notatation for Scalar product.

$$(\phi, \psi) \Rightarrow \langle\phi|\psi\rangle$$

matrix machanics notat.

$\langle r,t|\psi\rangle$

$$\Rightarrow \int \phi^*(r,t)\,\psi(r,t)\,d^3r$$

in wave machanics

$$(f,g) = \int_\alpha^\beta f(x)g(x)\,dx$$

for functionspace $\alpha \leq x \leq \beta$

$\hat{H}$ Scalar product

$(\phi, \hat{\psi}) \neq (\psi, \phi)$ → Not Commutative (because scalar ... is complex number)

$\langle \phi | \psi \rangle^* = \langle \psi | \phi \rangle$

In order to represent

$\langle \phi | \psi \rangle = \left(\int \phi^*(r,t) \psi(r,t) d^3r \right)^* = \int \phi(r,t) \psi^*(r,t) d^3r = \langle \psi | \phi \rangle$

Properties of Bra-ket Algebra

$|\psi\rangle \leftrightarrow \langle \psi |$

1. To every ket vector $|\psi\rangle$ there exist a unique bra vector $\langle \psi |$ and for every bra vector $\langle \psi |$ there corresponds to $|\psi\rangle$

$$a|\psi\rangle + b|\phi\rangle \longleftrightarrow a^* \langle \psi | + b^* \langle \phi | \quad ; \; a, b \text{ are complex number}$$

ket, bra

$$|a\psi\rangle = a|\psi\rangle \; ; \; \langle a\psi | \Rightarrow a^* \langle \psi |$$

2. Scalar product:-

$$\langle \psi | a_1 \psi_1 + a_2 \psi_2 \rangle = a_1 \langle \psi | \psi_1 \rangle + a_2 \langle \psi | \psi_2 \rangle$$

$$\langle a_1 \phi_1 + a_2 \phi_2 | \psi \rangle = a_1^* \langle \phi_1 | \psi \rangle + a_2^* \langle \phi_2 | \psi \rangle$$

$$\langle a_1 \phi_1 + a_2 \phi_2 | b_1 \psi_1 + b_2 \psi_2 \rangle = a_1^* b_1 \langle \phi_1 | \psi_1 \rangle + a_1^* b_2 \langle \phi_1 | \psi_2 \rangle + a_2^* b_1 \langle \phi_2 | \psi_1 \rangle + a_2^* b_2 \langle \phi_2 | \psi_2 \rangle$$

If Normalized ($\int \psi^* \psi d^3r$) wave [$\|f\| = \sqrt{(f,f)} = \sqrt{\int_a^b f(x)^2 dx}$, function space]

3. $\langle \psi | \psi \rangle = 1$ Normalization Condition ($\langle \psi | \psi \rangle = 0$ iff $|\psi\rangle = 0$)

4. Schwartz inequality: $|\langle \psi | \phi \rangle|^2 \leq \langle \psi | \psi \rangle \langle \phi | \phi \rangle$

(in vector space $|\vec{A} \cdot \vec{B}|^2 \leq |\vec{A}|^2 |\vec{B}|^2$, in Euclidian space)

5. Triangle Inequality.

$$\sqrt{\langle \psi + \phi | \psi + \phi \rangle} \leq \sqrt{\langle \psi | \psi \rangle} + \sqrt{\langle \phi | \phi \rangle}$$

$|\vec{A}| = \sqrt{A \cdot A}$ $\sqrt{A^2}$

$\vec{A}\cdot\vec{B} = AB$ Projection of B on A

$|\phi\rangle \cdot |\psi\rangle$ $\langle\phi|\psi\rangle$ = Projection of $|\psi\rangle$ on $|\phi\rangle$

$|\vec{A}+\vec{B}| \leq |\vec{A}| + |\vec{B}|$ triangle inequality

In Eucledian Space

6. Orthogonal states:-

$|\psi\rangle, |\phi\rangle$ to kets are of the same

$\langle\psi|\phi\rangle = 0$ vanishing scalar product

7) orthonormal. $(\phi_i, \phi_j) = \delta_{ij}$

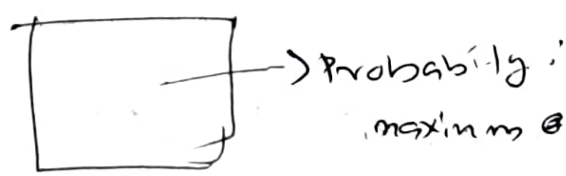
$\langle\psi|\phi\rangle = 0$ (orthogonal) & $\left.\begin{array}{l}\langle\psi|\psi\rangle = 1 \\ \langle\phi|\phi\rangle = 1\end{array}\right\}$ normalized

8. Forbidden Quantitys

$\left.\begin{array}{l}|\psi\rangle|\phi\rangle \\ \langle\psi|\langle\phi|\end{array}\right]$ Not allowed.

Normalization

$\langle\psi|\psi\rangle = 1$ or $\int_{-\infty}^{\infty} \psi^*\psi \, d^3r = 1$



eg: $\left.\begin{array}{l}|\psi\rangle = 3i|\phi_1\rangle - 7i|\phi_2\rangle \\ |\chi\rangle = -|\phi_1\rangle + 2i|\phi_2\rangle\end{array}\right]$ ϕ_1, ϕ_2 are orthonormal.

calculate.

1) $|\psi+\chi\rangle$ 2) $\langle\psi+\chi|$ 3) $\langle\psi|\chi\rangle$

4) $\langle\chi|\psi\rangle$ 5) show $|\psi\rangle, |\chi|$ obay shwartz eaequality & triagsuar inequality.

Ans.

1.) $|\psi+\chi\rangle = |\psi\rangle + |\chi\rangle$

$= (3i-1)|\phi_1\rangle - 5i|\phi_2\rangle$

2) $\langle\psi+\chi| = (3i-1)^*\langle\phi_1| - (5i)^*\langle\phi_2|$

$= (-3i-1)\langle\phi_1| + 5i\langle\phi|$

$=$

3. $\langle\psi|\chi\rangle \Rightarrow$ $\langle\phi_1|\phi_1\rangle = \langle\phi_2|\phi_2\rangle = 1$, $\langle\phi_1|\phi_2\rangle = \langle\phi_2|\phi_1\rangle = 0$] orthonormal

to bra

$\langle\psi| = (-3i\langle\phi_1| + 7i\langle\phi_2|)$

$|\chi\rangle (-|\phi_1\rangle + 2i|\phi_2\rangle)$

$\langle\psi|\chi\rangle = 3i\langle\phi_1|\phi_2\rangle + 14i^2\langle\phi_2|\phi_2\rangle$

$= 3i\langle\phi_1|\phi_2\rangle - 14\langle\phi_2|\phi_2\rangle$

$= 3i - 14$

$\langle\chi|\psi\rangle = \langle\psi|\chi\rangle^*$

$= -3i - 14$

shwartz inequality.

$|\langle\psi|\chi\rangle|^2 \leq \langle\psi|\psi\rangle\langle\chi|\chi\rangle$

$$|3i - 14|^2 \leq \langle\psi|\psi\rangle\langle\chi|\chi\rangle$$

$$3^2 + 14^2 \leq 58 \times 5$$ ✓

Triangular inequality

$$\sqrt{\langle\psi+\chi|\psi+\chi\rangle} \leq \sqrt{\langle\psi|\psi\rangle} + \sqrt{\langle\chi|\chi\rangle}$$

$$\left[-1-3i\langle\phi_1| + 5i\langle\phi_2|\right]\left[-1+3i|\phi_1\rangle - 5i|\phi_2\rangle\right]$$

$$= (-1-3i)(-1+3i) + (5i)(-5i)$$

$$= (1 - 3i + 3i + 9) + (+25) = 35$$

$$\leq \sqrt{58} \times \sqrt{5}$$

Operators $|\psi\rangle\hat{A}$, $\hat{A}\langle\phi|$ ⇒ not defind

Operator is a mathamatical rule that when applied to applied to ket $|\psi\rangle$ it transform it into another ket $|\psi'\rangle$ for same same and when it act on a bra $\langle\psi|$ transform it into another bra $\langle\psi'|$

$$\hat{A}|\psi\rangle = |\psi'\rangle \; ; \; \langle\phi|\hat{A} = \langle\phi'|$$

$\hat{A}\psi(r) = \psi'(r)$

example of operator are.

- unitary operator - it leaves any kets unchanged

$$\hat{I}|\psi\rangle = |\psi\rangle$$

Gradient operator $\nabla\psi(r) = \frac{\partial\psi}{\partial x}\hat{i} + \frac{\partial\psi}{\partial y}\hat{j} + \frac{\partial\psi}{\partial z}\hat{k}$

Linear momentum operator $\hat{p}\,\psi(r) = -i\hbar\nabla\psi(r)$

Laplacian operator $\nabla^2\psi(r) = \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}$

Parity operator $P\psi(r) = \psi(-r)$

Product of operator — think as a same matrix

$\hat{A}\hat{B} \neq \hat{B}\hat{A}$

$\hat{A}\hat{B}\hat{C} = \hat{A}(\hat{B}\hat{C}) = (\hat{A}\hat{B})\hat{C}$ → Associative

$\hat{A}\hat{B}\,|\psi\rangle = \hat{A}(\hat{B}|\psi\rangle)$ — The order doesn't matter — matter

Do it commt

$\langle\phi|\hat{A}|\phi\rangle$ = complex num / scalar

Any operator is said to be linear if it obeys distributive law

$$\hat{A}(a_1|\psi_1\rangle + a_2|\psi_2\rangle) = a_1\hat{A}|\psi_1\rangle + a_2\hat{A}|\psi_2\rangle$$

$$(\langle\psi_1|a_1 + \langle\psi_2|a_2)\hat{A} = a_1\langle\psi_1|\hat{A} + a_2\langle\psi_2|\hat{A}$$

Expectation value of $\langle\hat{A}\rangle$ (or mean value) of operate $\hat{A}$ wrt to $|\psi\rangle$

$$\langle\hat{A}\rangle = \frac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle}$$

$A|\psi\rangle$

$\langle\psi|A$

If not normal

Hermitian Adjoint or adjoint ($\hat{A}^\dagger$)

$$\langle\psi|\hat{A}^\dagger|\phi\rangle = \langle\phi|\hat{A}|\psi\rangle^*$$

Rules: $a^\dagger$ = ... $|\psi\rangle^\dagger$ or $\langle\phi|^\dagger$ replace

Hermitian (conjugate)

$$(\hat{A}^\dagger)^\dagger = \hat{A}$$

$$(a\hat{A})^\dagger = a^*\hat{A}^\dagger$$

$$(\hat{A}+\hat{B}+\hat{C}+\hat{D})^\dagger = \hat{A}^\dagger+\hat{B}^\dagger+\hat{C}^\dagger+\hat{D}^\dagger$$

$$(ABCD)^\dagger = \hat{D}^\dagger\hat{C}^\dagger\hat{B}^\dagger\hat{A}^\dagger \quad ((CD)^\dagger(AB)^\dagger)$$

$$(\hat{A}\hat{B}\hat{C}\hat{D}|\psi\rangle)^\dagger = \langle\psi|\hat{D}^\dagger\hat{C}^\dagger\hat{B}^\dagger\hat{A}^\dagger$$

Hermitian & skew Hermitian operators

Hermitian if

$\hat{A} = \hat{A}^\dagger$ or $\langle\psi|\hat{A}|\phi\rangle = \langle\phi|\hat{A}|\psi\rangle^*$

$\langle\psi|\hat{A}|\phi\rangle^\dagger = (\langle\psi|\hat{A}|\phi\rangle^*)^T$

skew hermitian or Antihermitian if

$\hat{B}^\dagger = -\hat{B}$ or $\langle\psi|\hat{B}|\phi\rangle = -\langle\phi|\hat{B}|\psi\rangle^*$

Projection operator

$\hat{P}$ said to be projection operator if it is hermitian its own square. ie

$\hat{P}^\dagger = \hat{P}$ and $\hat{P}^2 = P$.

eg. $\hat{I}$, $\hat{I}^\dagger = I$ or $\hat{I}^2 = I$

$|\phi\rangle\langle\psi|$ is a linear operator

eg: $|\phi\rangle\langle\psi|\psi'\rangle \Rightarrow \langle\psi|\psi'\rangle|\phi\rangle \Rightarrow$ a ket

inner product, complex number

$(|\psi\rangle\langle\phi|)^\dagger = |\phi\rangle\langle\psi|$

$|a\hat{A}\psi\rangle = a\hat{A}|\psi\rangle$; $\langle a\hat{A}\psi| = a^*\langle\psi|\hat{A}^\dagger$

note $\langle a\hat{A}^\dagger\psi| = a^*\langle\psi|\hat{A}$

Hence

$\langle\psi|\hat{A}|\phi\rangle = \langle\hat{A}^\dagger\psi|\phi\rangle = \langle\psi|\hat{A}\phi\rangle$

Commutator Algebra

measure simultaneously $\Rightarrow \hat{A}\hat{B}|\psi\rangle \Rightarrow \hat{B}\hat{A}|\psi\rangle$

$\hat{A}, \hat{B}$ $\quad [\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ - commutator

$\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ - Anticommutator

Two operator are said to be commute if their commutator is zero $[\hat{A}, \hat{B}] = 0 \Rightarrow \hat{A}\hat{B} = \hat{B}\hat{A}$

If two operator are Hermitian and their ~~their~~ product is also hermitian. then these operators commute.

$(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger = \hat{B}\hat{A}$ $\qquad \hat{A}^\dagger = A$, $\hat{B}^\dagger = B$

also $(\hat{A}\hat{B})^\dagger = \hat{A}\hat{B}$

$\hat{A}\hat{B} = \hat{B}\hat{A}$

$\Rightarrow [\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0$

eg.

$[\hat{X}, \hat{P}_x] = i\hbar \hat{I}$

$[\hat{Y}, \hat{P}_y] = i\hbar \hat{I}$

Properties of commutator

- Antisymmetry $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$

- Linearity

$$[\hat{A}, \hat{B} + \hat{C} + \hat{D} + \dots] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}] + [\hat{A}, \hat{D}] \dots$$

- Hermitian conjugate / adjoint of commutator:

$$[\hat{A}, \hat{B}]^{\dagger} = [B^{\dagger}, A^{\dagger}]$$

- Distributivity.

$$[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$$

$$[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$$

- Jacobi Identity

$$[\hat{A}, [\hat{B}, \hat{C}]] + [\hat{B}, [\hat{C}, \hat{A}]] + [\hat{C}, [\hat{A}, \hat{B}]] = 0$$

- Operator commute with scalar

$$[\hat{A}, b] = 0$$

we can take const out $\Rightarrow [\hat{A}, \frac{\hat{B}}{2}] \Rightarrow \frac{1}{2}[\hat{A}, \hat{B}]$

just expand

Q) Conside a state vector, $|\psi\rangle = \frac{1}{\sqrt{2}}|\phi_1\rangle + \frac{1}{\sqrt{5}}|\phi_2\rangle + \frac{1}{\sqrt{10}}|\phi_3\rangle$

which is given in terms of orthonormal eigen state $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle$ of an operato $\hat{B}$ such that

$\hat{B}|\phi_n\rangle = n^2|\phi_n\rangle$ find the expectation value of $\hat{B}$ for state $|\psi\rangle$

$\langle\psi| = |\psi\rangle$ since no $|\psi\rangle^T$

Ans - $\langle\hat{B}\rangle = \frac{\langle\psi|\hat{B}|\psi\rangle}{\langle\psi|\psi\rangle}$

$\langle\psi|\psi\rangle = \frac{1}{2} + \frac{1}{5} + \frac{1}{10}$

$= \frac{8}{10}$

$\langle\psi|\hat{B}|\psi\rangle = \left(\frac{1}{\sqrt{2}}\langle\phi_1| + \frac{1}{\sqrt{2}}\langle\phi_2| + \frac{1}{\sqrt{10}}\langle\phi_3|\right)\hat{B}\left(\frac{1}{\sqrt{2}}|\phi_1\rangle + \frac{1}{\sqrt{2}}|\phi_2\rangle + \frac{1}{\sqrt{10}}|\phi_3\rangle\right)$

$= \frac{1}{2}(1)^2\langle\phi_1|\phi_1\rangle + \frac{1}{5}2^2\langle\phi_2\phi_3\rangle + \frac{1}{10}3^2\langle\phi_3|\phi_3\rangle$

$\left(\hat{B}|\phi_n\rangle = n^2|\phi_n\rangle\right)$

$= \frac{22}{10}$

$\langle\hat{B}\rangle = \frac{22/10}{8/10} = \frac{11}{4}$

$[\hat{A}, \hat{B}+c] = \hat{A}\hat{B} + \hat{A}c - \hat{B}\hat{A} - \hat{A}c$

$= (\hat{A}, \hat{B})$

Matrix representation of ket, Bras and operators

Let us consider a ~~de~~discret, complete and orthonormal bases made up of infinite number of kets
$|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, \ldots, |\phi_n\rangle \rightarrow \{|\phi_n\rangle\}$ in Hilbert space

~~orthonormal~~ $\langle\phi_n|\phi_m\rangle = \delta_{nm} \rightarrow$ orthonormality.

$$\sum_{n=1}^{\infty} |\phi_n\rangle\langle\phi_n| = \hat{I}$$
unit operator

Matrix representation of kets state $|\psi\rangle$ in base $|\phi_n\rangle$

$$|\psi\rangle \Rightarrow \hat{I}|\psi\rangle = \sum_{n=1}^{\infty}\left(|\phi_n\rangle\langle\phi_n|\right)|\psi\rangle$$

$$|\psi\rangle = \sum_{n=1}^{\infty} a_n|\phi_n\rangle$$ where $a_n = \langle\phi_n|\psi\rangle$
like $\hat{i}\ \hat{j}\ \hat{k}$

the coe $\langle\phi_n|\psi\rangle = a_n$ projection of $|\psi\rangle$ on $|\phi_n\rangle$

$$|\psi\rangle \Rightarrow \begin{bmatrix} \langle\phi_1|\psi\rangle \\ \langle\phi_2|\psi\rangle \\ \vdots \\ \langle\phi_n|\psi\rangle \end{bmatrix} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_n \end{bmatrix}$$

, ~~so~~ kets are represented by column matrix.

With in th basis $\{|\phi_n\rangle\}$, The ket $|\psi\rangle$ is represented by set of it's components along $|\phi_1\rangle, \ldots |\phi_n\rangle$ respectively

The matrix representation of the bra vector $\langle\psi|$

$|\psi\rangle^{\dagger} = \langle\psi|$

$|\psi\rangle^{*} \neq \langle\psi|$

$$\langle\psi| = [\langle\psi|\phi_1\rangle \; \langle\psi|\phi_2\rangle \; \dots \; \langle\psi|\phi_n\rangle]$$

$$= [\langle\phi_1|\psi\rangle^* \; \langle\phi_2|\psi\rangle^* \; \dots \; \langle\phi_n|\psi\rangle^*]$$

$$= [a_1^* \; a_2^* \; \dots \; a_n^*]$$

bra $\langle\psi|$ can be represented by row matrix.

$$\langle\psi|\phi\rangle = [a_1 \cdots a_n] \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix} = \sum_n a_n b_n$$

$b_n = \langle\phi$

$a_n = \langle\psi$

matrix representation of operator.

$$\hat{A} = \hat{I}\hat{A}\hat{I} \Rightarrow \left[\sum_{n=1}^{\infty} |\phi_n\rangle\langle\phi_n|\right] \hat{A} \left[\sum_{m=1}^{\infty} |\phi_m\rangle\langle\phi_m|\right]$$

$$\Rightarrow \sum_{nm} A_{nm} |\phi_n\rangle\langle\phi_m| \; ; \; A_{nm} = \langle\phi_n|\hat{A}|\phi_m\rangle$$

→ elements of matrix of $\hat{A}$

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & \dots \\ A_{21} & A_{22} & \dots & \\ \vdots & \vdots & \ddots & \end{bmatrix}$$

without hat

Postulates of Qm

Classical mechanics → State of a system at any time t is specified by 2 dynamical variables. position an momentum.

Also State of system any later time t' can be predicted by hamiltonians eqn.

x, P at any time t,

$$\frac{dx}{dt} = \frac{\partial H}{\partial p} = \frac{\partial P}{\partial t} = \frac{-\partial H}{\partial x}$$

The QM counterparts of these ideas are specified by five different postulates.

Postulate - I ; State of system

State of any physical system at time T is specified by state vector $|\psi(t)\rangle$ in Hilbert space.

- state of a system can be represented by two or more wave functions linear combination

$$\psi(r,t) = \alpha_1 \psi_1(r_1,t_1) + \alpha_2 \psi_2(r_2,t)$$

Postulate = II ; Observable & operators

To every physical measurable quantity A (Observable or dynamical variables) there corresponds a linear Hermitian operator $\hat{A}$ whose eigen values form complete basis.

eg: Observable — operator

Position $\vec{r}$ — $\hat{R}$

$\vec{p}$ — $\hat{P} = -i\hbar\nabla$

$T = \frac{p^2}{2m}$ — $\hat{T} = \frac{-\hbar^2}{2m}\nabla^2$

$E = \frac{p^2}{2m} + V(r,t)$ — $\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + V(\hat{R},t)$

$\vec{L} = \vec{r} \times \vec{p}$ — $L = -i\hbar\hat{R}\times\nabla$

E for time dependence — $\hat{H} = i\hbar\frac{\partial}{\partial t}$

postulate-3 ; Measurements and Eigen values of operator

The measurement of an observable A may be represented by the action of operator A on state vector $|\psi(t)\rangle$

a_n is the component of $|\psi(t)\rangle$ on $|\psi_n\rangle$

$$\hat{A}|\psi(t)\rangle = a_n|\psi_n\rangle \quad ; \text{ where } a_n = \langle\psi_n|\psi(t)\rangle$$

a_n → Eigen value. (which is real)

$$\sum|\psi_n\rangle\langle\psi_n|\psi(t)\rangle \Rightarrow a_n|\psi_n\rangle$$

eigen basis ? - its

— Classically the process of measurement can be performed without disturbing the system. Significantly. However in QM the measurement process perturbs the system significantly.

$$h\nu = \frac{hc}{\lambda} = \frac{h \times 3\times10^8}{10^{-10}} \sim 10^4 eV$$



after measurements

Postulate-4 : Probabilistic outcome of the measurement

When measuring an observable A of system in the state $|\psi\rangle$ the probability of obtaining one of the ~~known~~ non degenerate eigen value ~~An is~~ (every eigenvector a unique eigenvalue) a_n of corresponding operator ~~is~~ $\hat{A}$ is given by

$$P_n(a_n) = \frac{|\langle\psi_n|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{|a_n|^2}{\langle\psi|\psi\rangle}$$

$|\psi_n\rangle$ eigen state of $\hat{A}$ operator with eigen value a_n

The act of measurement changes $|\psi\rangle$ to $|\psi_n\rangle$

P = square of the norm.

If the eigen value a_n is m fold degenerate

$$P_n(a_n) = \frac{\sum_{j=1}^{m} |\langle \psi_n^j | \psi \rangle|^2}{\langle \psi | \psi \rangle} = \frac{\sum_{j=1}^{m} |a_n^{(j)}|^2}{\langle \psi | \psi \rangle}$$

$$\boxed{\hat{A}|\psi\rangle = a_n|\psi_n\rangle}$$

Expectation value w.r.to $|\psi\rangle$

$$\langle \hat{A} \rangle = \frac{\langle \psi | \hat{A} | \psi \rangle}{\langle \psi | \psi \rangle}$$

avarage result of mesuring of Operator $\hat{A}$ on $|\psi\rangle$ state

$I \hat{A} I$

$$\langle \hat{A} \rangle = \frac{1}{\langle \psi | \psi \rangle} \sum_{nm} \langle \psi | \psi_m \rangle \langle \psi_m | \hat{A} | \psi_n \rangle \langle \psi_n | \psi \rangle$$

unitvector so no prob

$$= \sum_n a_n \frac{|\langle \psi_n | \psi \rangle|^2}{\langle \psi | \psi \rangle} \; ; \text{ where } \langle \psi_m | \hat{A} | \psi_n \rangle = a_n \delta_{mn}$$

$$\langle \hat{A} \rangle = \sum_n a_n \frac{|\langle \psi_n | \psi \rangle|^2}{\langle \psi | \psi \rangle} = \boxed{\sum_n a_n P_n} = \langle \hat{A} \rangle \quad P_n = \frac{|a_n|^2}{\langle \psi | \psi \rangle}$$

Eigen

$\sum$ eigen value × correspondi probability

Postulate 5: Time evolution of a system

Time evolution of the state vector $|\psi(t)\rangle$ is governed by the time dependend shrödinger eq^n

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla \psi + U\psi$$

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$

$E = \langle \hat{H} \rangle$

$H\psi = E\psi$

degenerate

$a_n|\psi_n\rangle$

result of measuring $\hat{A}$ on $|\psi\rangle$ state

$|\psi\rangle$

$\hat{A}|\psi_n\rangle = a_n \delta_{nm}$

$P_n = \frac{|a_n|^2}{\langle\psi|\psi\rangle}$

probability

for $|\psi(t)\rangle$

d end

Problem: Consider a state of system given in terms of a complete and orthonormal set of Φ vectors $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, |\phi_4\rangle, |\phi_5\rangle$ such that

$$|\psi\rangle = \frac{1}{\sqrt{19}}|\phi_1\rangle + \frac{2}{\sqrt{19}}|\phi_2\rangle + \sqrt{\frac{2}{19}}|\phi_3\rangle + \sqrt{\frac{3}{19}}|\phi_4\rangle + \sqrt{\frac{5}{19}}|\phi_5\rangle ;$$

where $|\phi_n\rangle$ are eigen state of Hamiltonian. $\hat{H}$

$\hat{H}|\phi_n\rangle = n\varepsilon_0|\phi_n\rangle$; $n = 1, 2, 3, 4 \ldots$, ε_0 have dimension of energy

a) Calculate the probability of finding the system in any one of the state $|\phi_n\rangle$ of one such system.

b) avg. energy of one such system (expectation value)

Ans: norm $\langle\psi|\psi\rangle = \sum_{n=1}^{5} a_n^2 \langle\phi_n|\phi_n\rangle$

$= \sum_{n=1}^{5} |a_n|^2 = \frac{1}{19} + \frac{4}{19} + \frac{2}{19} + \frac{3}{19} + \frac{5}{19}$

$= \frac{15}{19}$

Eigen value problem

$a_n =$

$E_n = \langle\phi_n|\hat{H}|\phi_n\rangle = n\varepsilon_0$, $E_1 = \varepsilon_0$, $E_2 = 2\varepsilon_0$, $E_3 = 3\varepsilon_0$, $E_4 = 4\varepsilon_0$, $E_5 = 5\varepsilon_0$

I think this is work

$\hat{H} = n\varepsilon_0 \langle\phi_n|\phi_n\rangle$

a) $P_1(E_1) = \frac{|\langle\phi_1|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \left|\frac{1}{\sqrt{19}}\langle\phi_1|\phi_1\rangle\right|^2 \times \frac{19}{15} = \frac{1}{15}$

$P_2(E_2) = \frac{|\langle\phi_2|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \left|\frac{2}{\sqrt{19}}\langle\phi_2|\phi_2\rangle\right|^2 \times \frac{19}{15} = \frac{4}{15}$

$P_3(E_3) = \frac{2}{15}$, $P_4(E_4) = \frac{3}{15}$, $P_5(E_5) = \frac{5}{15}$

b) $E = \sum_{j=1}^{5} P_j E_j = \ldots \rightarrow \langle \hat{H} \rangle \Rightarrow \sum a_n P_n$

$= \frac{1}{15} \times \varepsilon_0 + \frac{4}{15} 2\varepsilon_0 + \frac{2 \times 3\varepsilon_0}{15} + \frac{3 \times 4}{15} \varepsilon_0 + \frac{25}{15} \varepsilon_0$

$= \frac{52}{15} \varepsilon_0$

$E = \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{19}{15} \sum_{n=1}^{5} a_n^2 \langle \phi_n | \hat{H} | \phi_n \rangle$

$= \frac{19}{15} \left[\frac{1}{19}\varepsilon_0 + \frac{8}{19}\varepsilon_0 + \frac{6}{19}\varepsilon_0 + \frac{12}{19}\varepsilon_0 + \frac{25}{19}\varepsilon_0 \right] = \frac{52}{15}\varepsilon_0$

Probebility Dencity (only has physical meaning)

$P(r,t) = |\psi(r,t)|^2$, $\int_{-\infty}^{\infty} \psi^* \psi \, dr^3$ — scalar product

$= \int |\psi(r,t)|^2 dr^3 =$ If Normalized $= 1$

$\psi \Rightarrow$ finite, contineous, single valued, square integrable & derivatives

After measurement system will be on the eigen state of the operator

Before measuring an observeble a state $|\psi\rangle$ can represented by linear superposition of $|\phi_n\rangle$ of corresponding operator.

$|\psi\rangle = \sum_n |\phi_n\rangle\langle\phi_n|\psi\rangle = a_n |\phi_n\rangle$

The act of measurement change $|\psi\rangle$ to one of the eigenstat $|\psi_n\rangle$

If System is already in $|\psi_n\rangle$ measurments of the observable yields with certainity $(P=1)$ the value a_n without changing the state $|\psi_n\rangle$

Connection between QM & CM

Poisson braket & Commutator

$$\frac{1}{i\hbar}[\hat{A},\hat{B}] \rightarrow \{A,B\}_{classical}$$

reverse is not true.

Poisson braket between 2 dynamical variables A & B:
Poisson braket between 2 dynamical variable A & B
defind interms of Generalized coordinate
q_is and p_is of the system

$$\{A,B\} = \sum_j \left(\frac{\partial A}{\partial q_j}\cdot\frac{\partial B}{\partial p_j} - \frac{\partial A}{\partial p_j}\cdot\frac{\partial B}{\partial q_j}\right)$$

$\frac{\partial A}{\partial q_j}$ $\frac{\partial A}{\partial p_j}$
$\frac{\partial B}{\partial q_j}$ $\frac{\partial B}{\partial p_j}$

q_i are independent of p_is $\Rightarrow \frac{\partial q_j}{\partial p_k} = 0$; $\frac{\partial p_j}{\partial q_k} = 0$

$$\Rightarrow \{q_j, q_k\} = 0 = \{p_j, p_k\}$$

$$\{q_j, p_k\} = \delta_{jk}$$

$\frac{\partial q_j}{\partial q_j}\frac{\partial p_k}{\partial p_j} - \frac{\partial q_j}{\partial p_j}\frac{\partial p_k}{\partial q_j}$

CM is limiting case of QM

If 2 operator Commute

$[\hat{A},\hat{B}] = 0 \Rightarrow$ two operator commute

If two operator commute the both Quantities can be measured simutaniously at same time. to arbitary precision

$[\hat{A},\hat{B}] \neq 0 \Rightarrow$ It canot measure simultasiously.

$$\{A,B\}^* = \{A^*, B^*\}$$

Momentum operator position representation

$$\hat{p} = -i\hbar\nabla : \quad \hat{p}_x = -i\hbar\frac{\partial}{\partial x}, \quad \hat{p}_y = -i\hbar\frac{\partial}{\partial y}, \quad \hat{p}_z = -i\hbar\frac{\partial}{\partial z}$$

Just like Hamitonian (-ve sign)

Position operator in momentum representation

$$\hat{R}_j = i\hbar\frac{\partial}{\partial p_j}, \quad j = x, y, z \qquad \hat{x} = i\hbar\frac{\partial}{\partial p_x}, \quad \hat{y} = i\hbar\frac{\partial}{\partial p_y} \dots$$

Important Commutation relatio

$$[\hat{R}_j, \hat{p}_k] = ?$$

$$[x, p_x]\psi = ? \quad \hat{x}\hat{p}_x\psi - \hat{p}_x\hat{x}\psi \quad -① $$

$$\hat{x}\hat{p}_x\psi = x\left(-i\hbar\frac{\partial}{\partial x}\right)\psi = -i\hbar x\frac{\partial \psi}{\partial x}$$

$$\hat{p}_x\hat{x}\psi = -i\hbar\frac{\partial}{\partial x}(x\psi) = -i\hbar\psi - i\hbar x\frac{\partial \psi}{\partial x}$$

$$① \Rightarrow [\hat{x}, \hat{p}_x]\psi = i\hbar\psi$$

$$[\hat{x}, \hat{p}_x] = i\hbar \qquad \hat{z}\hat{p}_z = i\hbar$$

Similarly $[\hat{y}, \hat{p}_y] = i\hbar$

$$[\hat{x}, \hat{p}_y] = [\hat{x}, p_z] = [\hat{y}, \hat{p}_x] = [\hat{y}, p_z] = [\hat{z}, \hat{p}_x], [\hat{z}, \hat{p}_y] = 0$$

$$[\hat{R}_j, \hat{p}_k] = i\hbar\delta_{jk}$$

Similarly

$[\hat{x}^m, \hat{p}_x] = i\hbar m \hat{x}^{m-1}$

$\hat{x}^m p_x \psi = x^m i\hbar \frac{\partial \psi}{\partial x}$

$\hat{p}_x \hat{x}^m \psi = -i\hbar \frac{\partial}{\partial x}(x^m \psi) = \psi m x^{m-1} \ldots i\hbar$

$i\hbar m x^{m-1}$

Ehrenfest theorm

Time evolution of & position opeeration

expectation value of momentum

- we know that time evolution of $|\psi(t)\rangle$ of a system is govern by time depended shrödinger eqn

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \quad (1)$$

If QM is to be more general than CM then it must contain CM as a limiting case. To illustrate the idea, let us ~~take~~ look at the time evolution of expectation value of position & momentum operator $\vec{R}$ & $\vec{p}$ of a particle moving in a potential $V(r)$ ~~A~~ and compare with classical counterpart

$$(1) \Rightarrow \frac{d}{dt}|\psi(t)\rangle = \frac{1}{i\hbar}\hat{H}|\psi(t)\rangle \quad (2)$$

$$\frac{d}{dt}\langle\psi(t)| = \frac{-1}{i\hbar}\langle\psi(t)|\hat{H} \quad (3)$$

Time evolution of the expectation value of ~~an~~ a linear operator is given as

$$\langle\hat{A}\rangle = \langle\psi(t)|\hat{A}|\psi(t)\rangle$$

(again $|\psi\rangle$ normalized)

exp. value

$$\frac{d}{dt}\langle \hat{A}\rangle = \frac{d}{dt}\langle \psi(t)|\hat{A}|\psi(t)\rangle \quad -4$$

* product rule.

$$\frac{d}{dt}\left[\langle\psi|\hat{A}|\psi\rangle\right] = \left[\frac{d}{dt}\langle\psi|\right]\hat{A}|\psi\rangle + \langle\psi|\frac{d}{dt}(\hat{A})|\psi\rangle +$$

$$= \left[\frac{d}{dt}\langle\psi|\right]\hat{A}|\psi\rangle + \langle\psi|\left[\frac{d}{dt}(\hat{A}|\psi\rangle)\right]$$

$$= \left[\frac{d}{dt}\langle\psi|\right]\hat{A}|\psi\rangle + \langle\psi|\left[\frac{dA}{dt}|\psi\rangle + \hat{A}\frac{d}{dt}|\psi\rangle\right]$$

② & ③ in ⑤

$$\frac{d}{dt}\langle\psi|\hat{A}|\psi\rangle = \frac{-1}{i\hbar}\langle\psi|\hat{H}\hat{A}|\psi\rangle + \langle\psi|\frac{dA}{dt}|\psi\rangle + \frac{1}{i\hbar}\langle\psi|\hat{A}\hat{H}|\psi\rangle$$

* order

$$= \frac{1}{i\hbar}\langle\psi|\hat{A}\hat{H} - \hat{H}\hat{A}|\psi\rangle + \langle\psi|\frac{dA}{dt}|\psi\rangle \quad -⑥$$

$$\frac{d}{dt}\langle\hat{R}\rangle = ?\ ,\ \frac{d}{dt}\langle\hat{P}\rangle = ?$$

R & P donot depend on t explicitly

$$⑥ \quad \frac{d}{dt}\langle\hat{A}\rangle = \frac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle + \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle \quad -⑥$$

Position & momentum observable donot explicitly in the context of QM also $\left\langle\frac{\partial}{\partial t}X\right\rangle$ dependon time.

$$\left\langle\frac{d\hat{A}}{dt}\right\rangle = 0 \quad \hat{A},\ \hat{R} \,\&\, \hat{P}$$ (operator dont change overt)

$$⑥ \Rightarrow \frac{d}{dt}\langle\hat{A}\rangle = \frac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle \quad -⑦$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(R,t)$$

$$\frac{d}{dt}\langle \hat{R} \rangle = \frac{1}{i\hbar}\left\langle \left[\hat{R}, \frac{\hat{p}^2}{2m} + \hat{V}(R,t)\right] \right\rangle \quad \because \left[\hat{R}, \hat{V}(R,t)\right] = 0$$

$$= \frac{1}{i\hbar}\left\langle \left[R, \frac{p^2}{2m}\right] \right\rangle = \frac{1}{i\hbar 2m}\left\langle \left[R, \hat{p}^2\right] \right\rangle$$

$$\left[\hat{R}, \hat{p}^2\right] = 2i\hbar\hat{p}$$

$$\boxed{\frac{d}{dt}\langle \hat{R} \rangle = \frac{1}{m}\langle \hat{p} \rangle} \quad \text{— (8)}$$

$$\frac{d}{dt}\langle \hat{p} \rangle = \frac{1}{i\hbar}\left\langle \left[\hat{p}, \frac{p^2}{2m} + V(\hat{R},t)\right] \right\rangle$$

$$= \frac{1}{i\hbar}\left\langle \left[\hat{p}, \hat{V}(\hat{R},t)\right] \right\rangle$$

$$\left[\hat{P}, \hat{V}(\hat{R},t)\right] = -i\hbar\nabla\hat{V}(\hat{R},t)$$

check.

$$\boxed{\frac{d}{dt}\langle \hat{p} \rangle = -\langle \nabla V(\hat{R},t) \rangle} \quad \text{— (9)}$$

Ehrenfest Eqn

The respective forms in CM are

Hamiton - Jacobi eqn

$$\boxed{\frac{d\vec{r}}{dt} = \frac{\vec{p}}{m} \; ; \; \frac{dp}{dt} = -\vec{\nabla} V(\vec{r})}$$

$$\frac{dp}{dt} = m\frac{d^2r}{dt^2} = -\nabla V(r)$$ - reduce Newton, eqn

(8) & (9) there is no $\hbar$

$\lim_{\hbar \to 0}$ QM $\to$ CM , $\lim_{\lambda \to 0}$ $\to$ CM

$[\hat{R}, \hat{p}^2]\psi = \hat{R}\hat{p}^2\psi - \hat{p}^2\hat{R}\psi \Rightarrow \quad i\hbar\frac{\partial}{\partial p}p^2\psi - i\hbar p^2\frac{\partial}{\partial p}\psi$

$= i\hbar\left(\psi 2p + p^2\frac{\partial\psi}{\partial p} - p^2\frac{\partial\psi}{\partial p}\right)$

$[\hat{R}, \hat{p}^2] = i\hbar 2p\psi$

you can use $\frac{\partial}{\partial}c$ since ... 3D

$[\hat{p}, \hat{E}]\psi = \hat{p}\hat{E}\psi - \hat{E}\hat{p}\psi$

$-i\hbar\frac{\partial}{\partial x}\left(i\hbar\frac{\partial\psi}{\partial t}\right) + i\hbar\frac{\partial}{\partial t}\left(i\hbar\frac{\partial\psi}{\partial x}\right)$

$= \hbar^2\frac{\partial}{\partial x}\left(\frac{\partial\psi}{\partial t}\right) - \hbar^2\frac{\partial}{\partial t}\left(\frac{\partial\psi}{\partial x}\right) = 0$

$[\hat{p}, \hat{V}]\psi = \hat{p}\hat{V}\psi - \hat{V}\hat{p}\psi$

$= -i\hbar\frac{\partial}{\partial r}(V\psi) + i\hbar V\frac{\partial}{\partial r}\psi$

$= -i\hbar\left(\psi\frac{\partial V}{\partial r} + V\frac{\partial\psi}{\partial r} - V\frac{\partial\psi}{\partial r}\right)$

$= -i\hbar\nabla V(R,t)$ in 3D

$[\hat{R}, \hat{V}]\psi = RV - VR = 0$

operator

$\hat{A}|\psi\rangle = |\psi'\rangle$; $\langle\phi|\hat{A} = \langle\phi'|$

$\hat{A}\hat{B} \neq \hat{B}\hat{A}$

expectation value

$\langle\hat{A}\rangle \Rightarrow \dfrac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle}$

Hermitian adjoint

$\langle\psi|\hat{A}^{+}|\phi\rangle = \langle\phi|\hat{A}|\psi\rangle^{*}$ | $|\psi\rangle^{+} \Rightarrow \langle\psi|$; $a^{+} \Rightarrow a^{*}$

$(\hat{A}\hat{B})^{+} = \hat{B}^{+}\hat{A}^{-1}$

Hermitian

$\hat{A}^{+} = \hat{A} \Rightarrow \langle\psi|\hat{A}|\phi\rangle = \langle\phi|\hat{A}|\psi\rangle^{*}$

$\hat{A}^{+} = -\hat{B} \Rightarrow \langle\psi|\hat{A}|\phi\rangle = -\langle\phi|\hat{A}|\psi\rangle^{*}$

$\hat{P}^{+} = \hat{P}$ & $\hat{P}^{2} = \hat{P}$ Projection operator

---

$|a\hat{A}\psi\rangle \Rightarrow a\hat{A}|\psi\rangle$; $\langle a\hat{A}\psi| \Rightarrow a^{*}\langle\psi|A^{+}$

$\langle\psi A^{+}|\phi\rangle = \langle\psi|\hat{A}\phi\rangle$

$\Rightarrow \langle\psi|\hat{A}|\phi\rangle \Rightarrow$

Commutator Algebra

$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ | ant $\{\hat{A},\hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$

if commute $\Rightarrow [\hat{A},\hat{B}] = 0 \Rightarrow \hat{A}\hat{B} = \hat{B}\hat{A}$

$[\hat{A},\hat{B}] = -[\hat{B},\hat{A}]$, antisymmetric

$[\hat{A}, \hat{B} + \hat{C} + \hat{C} + \dots] \Rightarrow [\hat{A},\hat{B}] + [\hat{A},\hat{C}] + \dots$

$[\hat{A},\hat{B}]^{+} = [B^{+}, A^{+}]$

$[\hat{A},[\hat{B},\hat{C}]] + [\hat{B},[\hat{C},\hat{A}]] + [\hat{C},[\hat{A},\hat{B}]] = 0$, $\Rightarrow$ Jacobi identity

Scalar & operator commute

$[\hat{A}, b] = 0$

$\langle \phi_n | \phi_m \rangle = \delta_{mn} \Rightarrow \sum_{n=1}^{\infty} |\phi_n\rangle\langle\phi_n| = \hat{I}$

matrix

$|\psi\rangle$ on basis $|\phi_i\rangle$

$|\psi\rangle \Rightarrow \sum_{n=1}^{\infty} (|\phi_n\rangle\langle\phi_n|)|\psi\rangle$, $\langle\phi_n|\psi\rangle$ projection of $|\psi\rangle$ on $|\phi_n\rangle$

a_n

$|\psi\rangle = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} \langle\phi_1|\psi\rangle \\ \langle\phi_2|\psi\rangle \\ \langle\phi_n|\psi\rangle \end{bmatrix}$

$\langle\psi| = [\langle\phi_1|\psi\rangle^* \ \langle\phi_2|\psi\rangle^* \ \dots \ \langle\phi_n|\psi\rangle^*]$

$= [a_1^* \ a_2^* \ \ a_n^*]$

$\hat{A} = \hat{I}\hat{A}\hat{I} \Rightarrow \sum_{nm} A_{nm} |\phi_n\rangle\langle\phi_m|$, $A_{nm} = \langle\phi_n|\hat{A}|\phi_m\rangle$

$= \begin{pmatrix} A_{11} & A_{12} & \dots \\ A_{21} & A_{22} & \dots \\ \vdots & & \ddots \end{pmatrix}$

$a_n = \sum_n \langle\phi_n|\psi(t)\rangle$

Postulates of QM

eigen value

$\hat{A}|\psi_n\rangle = a_n|\psi_n\rangle$

eigen basis

$a_n \Rightarrow$ Component of $|\psi\rangle$ on $|\psi_n\rangle$

$E = \langle\hat{H}\rangle$

Probability

$P_n(a_n) = \frac{|\langle\psi_n|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{a_n^2}{\langle\psi|\psi\rangle}$

$\langle\hat{A}\rangle = \sum_n a_n P_n$ | $\langle\hat{A}\rangle = \frac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle}$

$\frac{1}{i\hbar}[\hat{A},\hat{B}] \rightarrow \{A,B\}$

$\{A,B\} = \sum_j \begin{vmatrix} \frac{\partial A}{\partial q_j} & \frac{\partial A}{\partial p_j} \\ \frac{\partial B}{\partial q_j} & \frac{\partial B}{\partial p_j} \end{vmatrix}$

$\{q_j\ q_k\} = \{p_j\ p_k\} = 0$

$\{q_j\ p_k\} = \delta_{jk}$

$\{A,B\}^* = \{A^*, B^*\}$

justik Heiz

$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$

$\hat{x} = i\hbar \frac{\partial}{\partial p_x}$

$[\hat{x}, \hat{p}_x] = i\hbar$

$[\hat{R}_j, \hat{P}_k] = i\hbar \delta_{jk}$

$\frac{d}{dt}\langle \hat{A} \rangle = \frac{1}{i\hbar}\langle [\hat{A}, \hat{H}] \rangle + \left\langle \frac{dA}{dt} \right\rangle$

$[\hat{x}^m, \hat{P}_x] = i\hbar m \hat{x}^{m-1}$

$[\hat{P}, \hat{E}] = 0$

$[\hat{P}, V] = -i\hbar \nabla V(R,t)$

$[R, V] = 0$

Ehrenfest theor

$\frac{d}{dt}\langle \hat{R} \rangle = \frac{1}{m}\langle \hat{P} \rangle$

$\frac{d}{dt}\langle \hat{P} \rangle = -\langle \nabla V(R,t) \rangle$

Potential step

$E > V_0$

$(e^{-i\omega t})$ for $\psi(x,t)$



$\psi_{1(x)} = Ae^{ik_1 x} + Be^{-ik_1 x}$, $k_1 = \frac{\sqrt{2mE}}{\hbar}$

$\psi_{2(x)} = Ce^{ik_2 x} + De^{-ik_2 x}$, $D = 0$

$k_2 = \frac{\sqrt{2m(E-V)}}{\hbar}$

$R_{\text{reflected}} = \left| \frac{J_{\text{reflected}}}{J_{\text{incident}}} \right| \Rightarrow \frac{|B|^2}{|A|^2}$, $T = \left| \frac{J_{\text{transmitted}}}{J_{\text{incident}}} \right| = \frac{|C|^2}{|A|^2} \frac{k_2}{k_1}$

$J_{inc} = \frac{i\hbar}{2m}\left(\psi_i(x) \frac{d\psi_i^*(x)}{dx} - \psi_i^* \frac{d\psi_i(x)}{dx} \right) = \frac{\hbar k_1}{m}|A|^2$

$\Rightarrow J_{\text{reflected}} = -\frac{\hbar k_1}{m}|B|^2$, $J_{tra} = \frac{\hbar k_2}{m}|C|^2$

Boundary condition $\Rightarrow$

$A + B = C$

$(A - B)k_1 = Ck_2$

$B = \frac{k_1 - k_2}{k_1 + k_2} A$, $C = \frac{2k_1}{k_1 + k_2} A$

$\Rightarrow R = \frac{(1-K)^2}{(1+K)^2}$, $K = \frac{k_1}{k_2}$, $K = \sqrt{1 - \frac{V_0}{E}}$

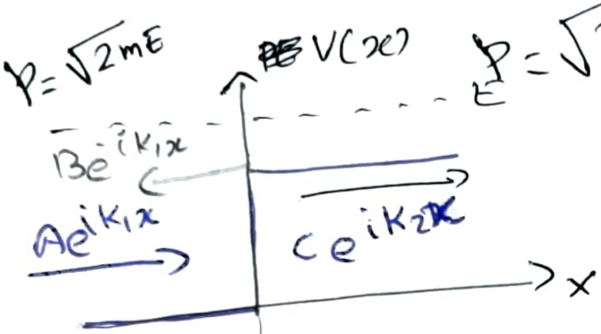
$T = \frac{4K}{(1+K)^2} \Rightarrow R + T = 1$

Application of Shrödiger wave eqn

Energy of Incident > Potential barrier

① Potential Step

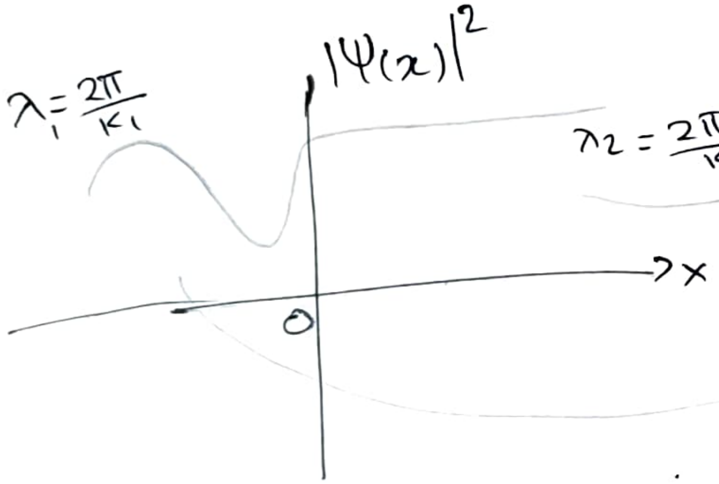
$p = \sqrt{2mE}$ $\quad p = \sqrt{2m(E-V_0)}$



$$V(x) = \begin{cases} 0, & x < 0 \\ V_0, & x \geq 0 \end{cases} \quad -①$$

P = momentum.

Particle come from left



$\psi^* \psi$

$Ce^{-ik_2x} \times Ce^{ik_2x} = C^2 e^0 = C$

$(Ae^{-ik_1x} + Be^{ik_1x})(Ae^{ik_1x} + Be^{-ik_1x})$

=

Case I $\quad E > V_0$ (For flux of particles)

let $\psi = Ce^{\lambda x}$

$\frac{d^2\psi}{dx^2} = \psi \lambda^2$

② $\rightarrow \lambda^2 \psi + k_1^2 \psi$

$\psi(\lambda^2 + k^2)$

$\lambda = \pm ik$

$C_1 e^{ikx} + C_2 e^{-ikx}$

$$\left(\frac{d^2}{dx^2} + k_1^2\right) \psi_1(x) = 0 \quad x < 0 \quad -②$$

$$\left(\frac{d^2}{dx^2} + k_2^2\right) \psi_2(x) = 0 \quad x \geq 0 \quad -③$$

$k_1^2 = \frac{2mE}{\hbar^2}$ $\qquad k_2^2 = \frac{2m(E-V_0)}{\hbar^2}$ — (4)

most are plane waves

$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$ — (5) ; $x<0$

$\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}$ — 0 — (6) $x>0$

Complete wave function can be written,

$$\psi(x,t) = \begin{cases} \psi_1(x)e^{-i\omega t} = Ae^{i(k_1x-\omega t)} + Be^{-i(k_1x-\omega t)} \\ \psi_2(x)e^{-i\omega t} = Ce^{i(k_2x-\omega t)} \end{cases} \quad -(7)$$

Reflection & Transmission Coeffients

$R = \frac{\text{reflected current dencity}}{\text{Incident current dencity}}$ or $R = \left| \frac{J_{reflected}}{J_{incident}} \right|$

$J_{incid} = \frac{\hbar}{2im}\left(\psi_i^*(x)\frac{d\psi_i(x)}{dx} - \psi_i(x)\frac{d\psi_i^*(x)}{dx}\right)$

ψ_i = incident

ψ_t = trans

$J_{inc} = \frac{\hbar k_1}{m}|A|^2$

$J_{ref} = -\frac{\hbar k_1}{m}|B|^2$

$J_{tran} = \frac{\hbar k_2}{m}|C|^2$

$J(x,t) = \frac{i\hbar}{2m}\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right)$

$\frac{i\hbar}{2m}\nabla(\psi^*\psi)$

$$\Rightarrow R = \left|\frac{J_{reflected}}{J_{inc}}\right| = \frac{|B|^2}{|A|^2} \quad \text{— (12)}$$

$$T = \left|\frac{J_{tran}}{J_{inc}}\right| = \frac{k_2}{k_1}\frac{|C|^2}{|A|^2} \quad \text{— (13)}$$

Calculation of R&T Reduced to Calculation of B&C for this

Boundary condition

Both wave function and it's derivatives are continuous at $x=0$

$$\psi_1(0) = \psi_2(0) \;;\; \frac{d\psi_1(0)}{\partial x} = \frac{\partial \psi_2(0)}{\partial x} \quad \text{— (14)}$$

Using these Boundary Condition (5) & (6)

$e^0 = 1$ $\qquad$ $Aik_1e^0 - Bik_1e^0 = Cik_2e^0$

$$A + B = C \quad \text{— (i)} \qquad k_1(A - B) = k_2 C \quad \text{— (ii)}$$

$\Downarrow$

$$B = \frac{k_1 - k_2}{k_1 + k_2}A \qquad C = \frac{2k_1}{k_1 + k_2}A \quad \text{— (15)}$$

$$\Rightarrow R = \frac{B^2}{A^2} = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} \quad \boxed{\frac{(1 - K)^2}{(1 + K)^2} = R} \quad \text{— (16)}$$

$$K = \frac{k_2}{k_1} = \sqrt{1 - \frac{V_0}{E}}$$

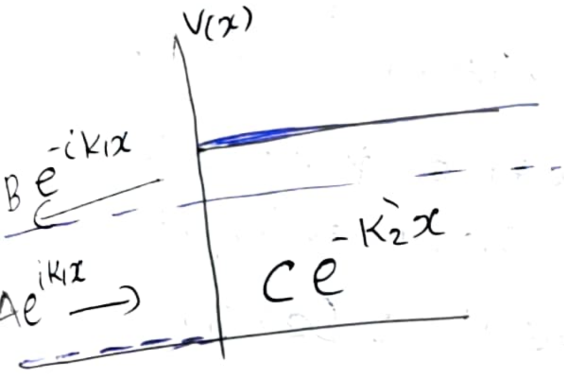
$$\Rightarrow T = \frac{k_2|C|^2}{k_1|A|^2} = \frac{4k_1^2 k_2}{(k_1 + k_2)^2} = \boxed{T = \frac{4K}{(1 + K)^2}} \quad \text{— (17)}$$

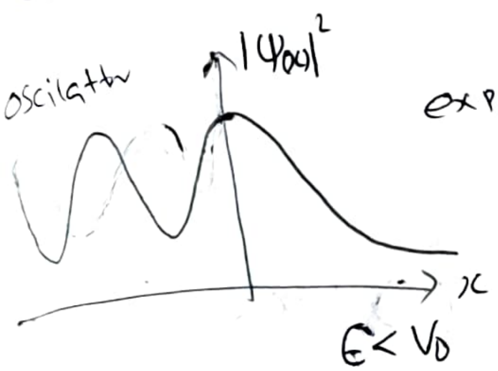
$$\Rightarrow \boxed{R + T = 1}$$

here is a finite probability of ~~refl~~ ~~a refraction~~ reflection
of particle back (ψ :: $R \neq 0$), unlike cm

this is attributed to the wavelike behavior of the incident particle. even though Energy is higher

Case-II $E < V_0$; $V(x) \begin{cases} 0 & ; x < 0 \\ V_0 & ; x \geq 0 \end{cases}$





exponential decay.

Particle wave (-ve outside)

$$\left(\frac{d^2}{dx^2} - k_2'^2\right)\psi_2(x) = 0$$

$\times e^{-i\omega t} \Rightarrow \psi(x,t)$

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \quad ; x < 0 \quad \text{— (18)}$$

$$\psi_2(x) = Ce^{-k_2'x} + De^{k_2'x} \quad ; x \geq 0$$

($De^{k_2'x}$: non-i, Diverge ✗)

$$k_2'^2 = 2m(V_0 - E)/\hbar^2$$

$$J_{transmitted} = \frac{\hbar}{2im}\left(\psi_t^*(x)\frac{d\psi_t(x)}{dx} - \psi_t(x)\frac{d\psi^*(x)}{dx}\right) = 0$$

$\psi(t)$ real

$\psi_t = Ce^{-k_2 x} = \psi_t^*$

$\Rightarrow J_{tran} = 0 \qquad = T = \left|\frac{J_{tran}}{J_{inc}}\right| = \frac{0}{J_{inc}} = 0$

$R = 1$

$(R+T) = 1$

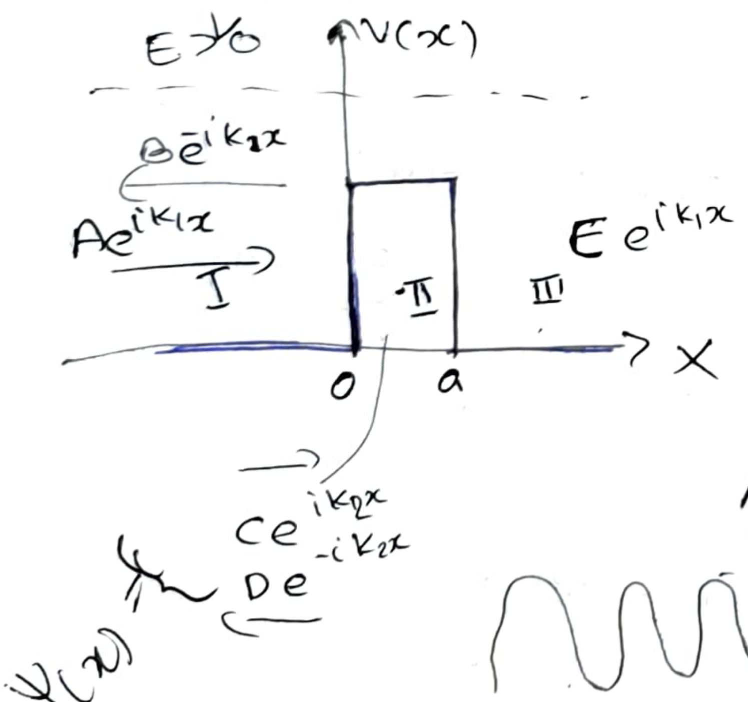
$$P = |\psi_t(x)|^2 = |C|^2 e^{-2k_2 x}$$

— Probability of finding the particle in second region is finite

although the energy of the particle is lower than the potential barrier hight

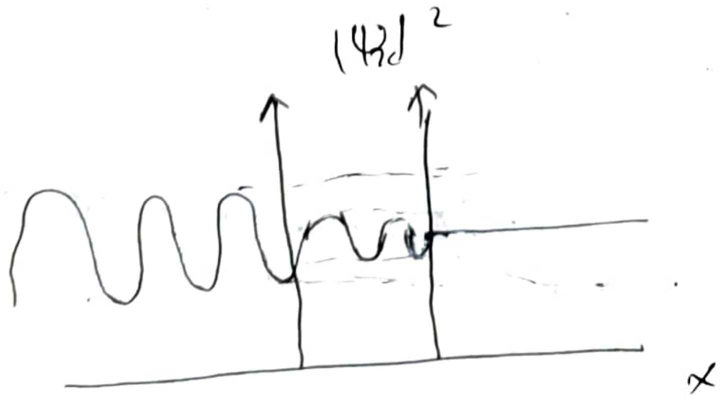
This is attributed to wave like behaviour of incident particle.

Potential barrier



$$V(x) = \begin{cases} 0 \,; & x < 0 \\ V_0 \,; & 0 \le x \le a \\ 0 \,; & x > a \end{cases}$$

total transmission



$+\frac{0}{\sin c} = 0$

$+T) = 1$

bability of finding the parti(cle) in second region is finite

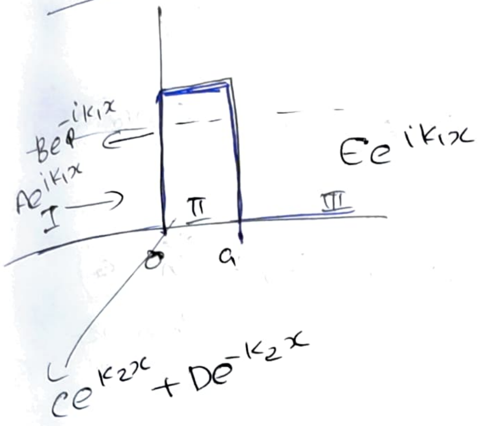
the particle is lower
barrier hight
like behaviour of

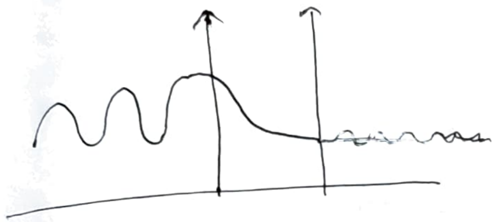
$= \begin{cases} 0 \; ; x < 0 \\ V_0 \; ; 0 \le x \le a \\ 0 \; ; x > a \end{cases}$

total transmission

x

E< V0





Boundary condition

$\psi_1(0) = \psi_2(0)$ & $\frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx}$

$\psi_2(a) = \psi_3(a)$ & $\frac{d\psi_2(a)}{dx} = \frac{d\psi_3(a)}{dx}$

$A + B = C + D.$

$ik_2(A_2 - A_1) = ik_2(C - D)$

$$\psi(x) = \begin{cases} \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \; ; x \le 0 \\ \psi_2(x) = Ce^{ik_2x} + De^{-ik_2x} \; ; 0 < x < a \\ \psi_3(x) = Ee^{ik_1x} \; ; x \ge 0 \end{cases}$$

E ≥ V0

Assignment

Assignment

1) Calculate R&T For. Enegy $E<V_0$ $E>V_0$

2) Calculate the Enersy of Particles with $E>V_0$ at totel transmission. (when $T=1$

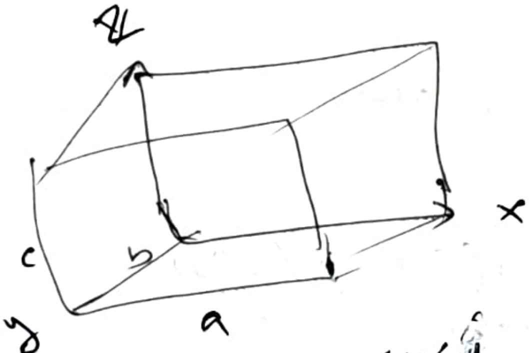
3) ST For Enegy $E<V_0$ at classical limit ($\hbar \to 0$)

$ka \to 0$

$R \sim 1$

$T \sim 0$

Box potential



$$V(x,y,z) = \begin{cases} 0 \; ; & 0<x<a; \quad 0<y<b \quad 0<z<c \\ \infty \; ; & \text{else where} \end{cases}$$

which canbe written as $V_x(x) + V_y(y) + V_z(z)$

$$V_x(x) = \begin{cases} 0 \; ; & 0<x<a \\ \infty \; ; & \text{elsewhere} \end{cases}$$

; $V_y y$; $V_z z$ have similer form

we know that $X(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n_x \pi}{a} x\right)$ — (1)

$$Y(y) = \sqrt{\frac{2}{b}} \sin\left(\frac{n_y \pi}{b} y\right)$$

1D box

$$Z(z) \; \sqrt{\frac{2}{c}} \sin\left(\frac{n_z \pi}{c} z\right)$$

$$\psi_{n_x n_y n_z}(x,y,z) = X_{(x)} Y_{(y)} Z_{(z)} = \sqrt{\frac{8}{abc}} \sin\left(\frac{n_x\pi}{a}x\right)\sin\left(\frac{n_y\pi}{b}y\right)\sin\left(\frac{n_z\pi}{c}z\right)$$

In 1D

$$E_{n_x} = \frac{\hbar^2\pi^2 n_x^2}{2ma^2}$$

$$E_{n_y} = \frac{\hbar^2\pi^2 n_y^2}{2mb^2}$$

$$E_{n_z} = \frac{\hbar^2\pi^2 n_z^2}{2mc^2}$$

$$E_{n_x n_y n_z} = E_{n_x} + E_{n_y} + E_{n_z} = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$$

~~If A=B~~ If symmetric $a=b=c=L$

Cubic box

$$\Rightarrow E_{n_x n_y n_z} = \frac{\hbar^2\pi^2}{2mL^2}(n_x^2+n_y^2+n_z^2)$$

For ground state energy $(n_x = n_y = n_z = 1)$

$$E_{111} = \frac{3\hbar^2\pi^2}{2mL^2} \Rightarrow E_{111} = 3E_1$$

(zeropont energy.

Exited state Enegys ψ_{211}

First exitedstate.

$n_x n_y n_z = (2,1,1),(1,2,1),(1,1,2)$

3 fold degenerate

$$E_{211} = E_{121} = E_{112} = \frac{6\pi^2\hbar^2}{2mL^2} = 6E_1$$

$$\psi_{211} = \sqrt{\frac{8}{L^3}} \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{\pi}{L} y\right) \sin\left(\frac{\pi}{L} z\right)$$

$$\psi_{121} = \sqrt{\frac{8}{L^3}} \sin\left(\frac{\pi}{L} x\right) \sin\left(\frac{2\pi}{L} y\right) \sin\left(\frac{\pi}{L} z\right)$$

$$\psi_{112} = \sqrt{\frac{8}{L^3}} \sin\left(\frac{\pi}{L} x\right) \sin\left(\frac{\pi}{L} y\right) \sin\left(\frac{2\pi}{L} z\right)$$

Second excited state

$(n_x n_y n_z) = (221), (212), (122)$ — 3 fold degenerated

$$E_{221}, E_{122}, E_{122} = \frac{9\pi^2 \hbar^2}{2mL^2} = 9E_1$$

$(n_x n_y n_z)$	$(E_{n_x n_y n_z})$ in E_1	g_n degenerate
(111)	$3E_1$	1
(211)(121)(112)	$6E_1$	3
(221)(212)(122)	$9E_1$	3
(311)(131)(113)	$11E_1$	3
(222)	$12E_1$	1
(321)(312)(231)(213)(132)(123)	$14E_1$	6

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$$

Symmetry leads to degeneracy in quantum system.

(Only cubic have symmetry not for box)

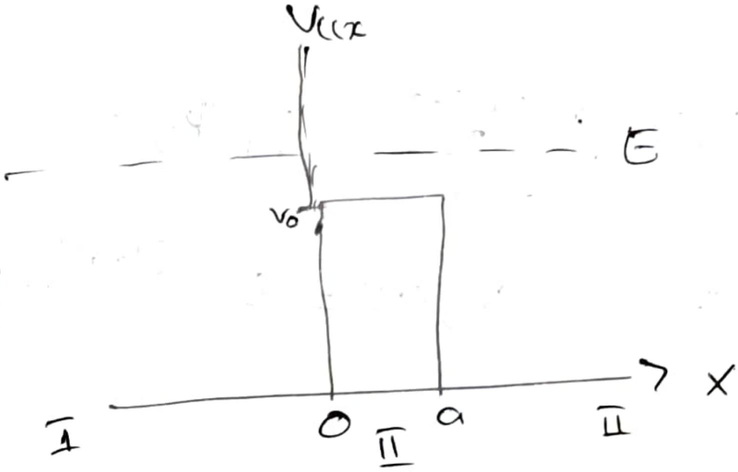
Due to symmetry

1) Calculate the R & T for $E < V_0$ and $E > V_0$ for potential barriers

Beam of particle with energy E and mass m' that are send from the left of potential barriers.

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 \leq x \leq a \\ 0 & x > a \end{cases}$$

Case 1 $E > V_0$



Shrödinger equation of the particle at different regions

$$\frac{\partial^2 \psi_1(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - U)\psi(x) = 0$$

I ⇒ $\psi_1(x)$, $U = 0$

$$\frac{d^2\psi_1(x)}{dx^2} + \frac{2mE}{\hbar}\psi_1(x) = 0$$

Let $\frac{2mE}{\hbar} = K_1^2$

$$\frac{d^2\psi_1(x)}{dx^2} + K_1^2\psi_1(x) = 0$$

Assume $\psi_1(x) = Ce^{\alpha x}$

$$\frac{d^2\psi_1(x)}{dx^2} = \alpha^2 Ce^{\alpha x} = \alpha^2\psi_1(x)$$

⇒

$$\alpha^2\psi_1(x) + K_1^2\psi_1(x) = 0$$

$$\alpha^2 = -K_1^2 \Rightarrow \alpha = \pm iK_1$$

General solution ⇒ $C_1 e^{iK_1 x} + C_2 e^{-iK_2 x}$

$$\Rightarrow \psi_1(x) = Ae^{iK_1 x} + Be^{-iK_2 x}$$

Similarly Shrodinger equation for II & III are

II $\frac{d^2\psi_2(x)}{d(x)^2} + K_2\psi_2(x) = 0$, $K_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$

G.S ⇒ $\psi_2(x) = Ce^{iK_2x} + De^{-iK_2x}$

III ⇒ $\frac{d^2\psi_3(x)}{dx^2} + K_1\psi_3(x) = 0$ $K_1 = \frac{\sqrt{2mE}}{\hbar}$

G.S = $\psi_3(x) = Ee^{iK_1x} + Fe^{-iK_1x}$ → 0, since there is no Boundary to reflect b

$$\psi(x) = \begin{cases} \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} & x \leq 0 \\ \psi_2(x) = Ce^{ik_2x} + De^{-ik_2x} & 0 < x < a \\ \psi_3(x) = Ee^{ik_1x} & x \geq a \end{cases}$$

In order to Find A, B, C, D, we know that wave function & its derivatives are continuous Boundary Conditions.

⇒ $\psi_1(0) = \psi_2(0)$, $\frac{d\psi_1(x)}{dx} = \frac{d\psi_2(x)}{dx}$ — ①

$\psi_2(a) = \psi_3(a)$ $\frac{d\psi_2(a)}{dx} = \frac{d\psi_3(a)}{dx}$ — ②

① ⇒ $A + B = C + D$ $(e^0 = 1)$

$\frac{d\psi_1(x)}{dx} = ik_1Ae^{ik_1x} - ik_1Be^{-k_1x}$

$$\frac{d\psi_2(x)}{dx} = ik_2 C e^{ik_2 x} - ik_2 D e^{-ik_2 x}$$

$(x=0)$

$$ik_1 A - ik_1 B = ik_2 C - ik_2 D$$

$$ik_1 (A-B) = ik_2 (C-D)$$

$(x=a)$

② ⇒ $$C e^{ik_2 a} + D e^{-ik_2 a} = E e^{ik_1 a}$$

$$ik_2 (C e^{ik_2 a} - D e^{-ik_2 a}) = ik_1 E e^{ik_1 a}$$

Solving for E, we obtain

$$E = 4k_1 k_2 A e^{-ik_1 a} \left[(k_1+k_2)^2 e^{-ik_2 a} - (k_1-k_2)^2 e^{ik_2 a} \right]^{-1}$$

$$= 4k_1 k_2 A e^{-ik_1 a} \left[4k_1 k_2 \cos(k_2 a) - 2i(k_1^2+k_2^2) \sin(k_2 a) \right]^{-1}$$

The transmission is given by

$$T = \frac{k_1 |E|^2}{k_1 |A|^2} = \left[1 + \frac{1}{4} \left(\frac{k_1^2 - k_2^2}{k_1 k_2} \right)^2 \sin^2(k_2 a) \right]^{-1}$$

$$T = \left[1 + \frac{V_0^2}{4E(E-V_0)} \sin^2 \left(a \sqrt{(2mV_0/\hbar^2)} \sqrt{(E/V_0)-1} \right) \right]^{-1}$$

~~because $\left(\frac{k_1^2 - k_2^2}{k_1 k_2} \right)^2 = \frac{V_0}{E(E-V_0)}$~~

~~Using the notation $\lambda = a\sqrt{2mV_0/\hbar^2}$ and $\varepsilon = E/V_0$~~

~~we can write.~~

$$T = \left[1 + \frac{1}{4\varepsilon(\varepsilon-1)} \sin^2(\lambda\sqrt{\varepsilon-1})\right]^{-1}$$

Similarly

$$R = \left[\frac{\sin^2(\lambda\sqrt{\varepsilon-1})}{4\varepsilon(\varepsilon-1)+\sin^2(\lambda\sqrt{\varepsilon-1})}\right] = \left[1 + \frac{4\varepsilon(\varepsilon-1)}{\sin^2(\lambda\sqrt{\varepsilon-1})}\right]^{-1}$$

Case $E < V_0$

$$\psi(x) = \begin{cases} \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} & x \le 0 \\ \psi_2(x) = Ce^{k_2x} + De^{-k_2x} & 0 < x < a \\ \psi_3(x) = Ee^{ik_1x} & x > a \end{cases}$$

where $k_1^2 = 2mE/\hbar^2$ and $k_2^2 = 2m(V_0-E)/\hbar^2$

Shrödinger eqn for II

$$\frac{d^2\psi_2(x)}{dx^2} - k_2\psi_2(x) = 0$$

let $\psi = Ce^{\lambda x}$

$$\lambda^2\psi_2 - k_2\psi_2 = 0$$

$$\lambda^2 = k_2$$

$$\lambda = \pm k_2$$

as $\psi_2(x) = Ce^{k_2x} + De^{-k_2x}$

$$R = \frac{|B|^2}{|A|^2}, \quad T = \frac{|E|^2}{|A|^2}$$

Boundary condition ⇒

$$A + B = C + D \quad -(1)$$

$$ik_1(A-B) = k_2(C-D) \quad -(2)$$

$$Ce^{k_2a} + De^{-k_2a} = Ee^{ik_1a} \quad -(3)$$

$$k_2(Ce^{k_2a} - De^{-k_2a}) = ik_1Ee^{ik_1a} \quad -(4)$$

$C = \frac{E}{2}\left(1 + i\frac{k_1}{k_2}\right)e^{(ik_1 - k_2)a}$, $D = \frac{E}{2}\left(1 + i\frac{k_1}{k_2}\right)e^{(ik_1 + k_2)a}$

(from last two expressions)

inserting these two equations in ① & ② and divide by A

$$1 + \frac{B}{A} = \frac{E}{A}e^{ik_1a}\left[\cosh(k_2a) - i\frac{k_1}{k_2}\sinh(k_2a)\right]$$

$$1 - \frac{B}{A} = \frac{E}{A}e^{ik_1a}\left[\cosh(k_2a) + i\frac{k_2}{k_1}\sinh(k_2a)\right]$$

solving these two equations for B/A & E/A

$$\frac{B}{A} = -i\frac{k_1^2 + k_2^2}{k_1 + k_2}\sinh(k_2a)\left[2\cosh(k_2a) + i\frac{k_2^2 - k_1^2}{k_1k_2}\sinh(k_2a)\right]^{-1}$$

$$\frac{E}{A} = 2e^{-ik_1a}\left[2\cosh(k_2a) + i\frac{k_2^2 - k_1^2}{k_1k_2}\sinh(k_2a)\right]^{-1}$$

Thus the coeffients R&T become

$$R = \left(\frac{k_1^2 + k_2^2}{k_1k_2}\right)^2\sinh^2(k_2a)\left[4\cosh^2(k_2a) + \left(\frac{k_2^2 - k_1^2}{k_1k_2}\right)^2\sinh^2(k_2a)\right]^{-1}$$

$$T = \frac{|E|^2}{|A|^2} = 4\left[4\cosh^2(k_2a) + \left(\frac{k_2^2 - k_1^2}{k_1k_2}\right)^2\sinh^2(k_2a)\right]^{-1}$$

we can rewrite R in term of T as.

$$R = \frac{1}{4}T\left(\frac{k_1^2 + k_2^2}{k_1k_2}\right)^2\sinh^2(k_2a)$$

Since $\cosh^2(k_2a) = 1 + \sinh^2(k_2a)$

$$T = \left[1 + \frac{1}{4}\left(\frac{k_1^2 + k_2^2}{k_1 k_2}\right)^2 \sinh^2(k_2 a)\right]^{-1}$$

This is known as tunneling effect.

2) calculate the Energy of the particle with $E > V_0$ at totel transmission $(T = 1)$

in the limit $\varepsilon \to 1$ we have $\sin(\lambda\sqrt{\varepsilon - 1}) \sim \lambda\sqrt{\varepsilon - 1}$ hence

$$T = \left(1 + \frac{m a^2 V_0}{2\hbar}\right)^{-1}, \quad R = \left(1 + \frac{2\hbar}{m a^2 V_0}\right)^{-1}$$

$$T = \left[1 + \frac{V_0^2 \sin^2 k_2 a}{4E(E - V_0)}\right]^{-1}$$

$\sin(a) = n\pi$

we have totel transmission when $\sin(\lambda\sqrt{\varepsilon - 1}) = 0$

or $\lambda\sqrt{\varepsilon - 1} = n\pi$, $\lambda = \frac{a\sqrt{2mV_0}}{\hbar}$ & $\varepsilon = E/V_0$

$$\Rightarrow \frac{a\sqrt{2mV_0}}{\hbar}\sqrt{\frac{E}{V_0} - 1} = n\pi$$

$$\frac{\sqrt{2m(E - V_0)}}{\hbar} = \frac{n\pi}{a} \quad \text{squaring}$$

$$E = V_0 + \frac{n^2\pi^2\hbar^2}{2ma^2}, \quad n = 1, 2, 3, 4 \ldots$$

Show that for $E < V_0$ at classical limit (...) $R \to 1$ & $T \to 0$

from the ~~eq~~ equation of T

$\sinh^2(k_2 a) = 0$, $k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

at classical limit $\hbar \to 0$ $\Rightarrow k_2 \to \infty$

$\Rightarrow T = [\infty]^{-1} = 0$

when $T = 0$, $R = 1$ $[R + T = 1]$

justik Hen

$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$

$\hat{x} = i\hbar \frac{\partial}{\partial p_x}$

$[\hat{x}, \hat{p}_x] = i\hbar$

$[\hat{x}^m, \hat{p}_x] = i\hbar m \hat{x}^{m-1}$

$[\hat{R}_j, \hat{P}_k] = i\hbar \delta_{jk}$

$\frac{d}{dt}\langle \hat{A} \rangle = \frac{1}{i\hbar}\langle [\hat{A}, \hat{H}] \rangle + \left\langle \frac{dA}{dt} \right\rangle$

Ehrenfest theorem

$\frac{d}{dt}\langle \hat{R} \rangle = \frac{1}{m}\langle \hat{P} \rangle$

$\frac{d}{dt}\langle \hat{P} \rangle = -\langle \nabla V(R,t) \rangle$

$[\hat{P}, \hat{E}] = 0$

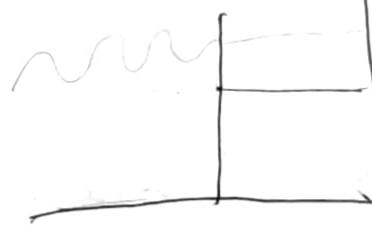
$[\hat{P}, V] = -i\hbar \nabla V(R,t)$

$[R, V] = 0$

Potential step

$E > V_0$

$e^{-i\omega t}$ for $\psi(x,t)$



$\psi_{1(x)} = Ae^{ik_1 x} + Be^{-ik_1 x}$, $k_1 = \frac{\sqrt{2mE}}{\hbar}$

$\psi_{2(x)} = Ce^{ik_2 x} + De^{-ik_2 x}$ ($D = 0$), $k_2 = \frac{\sqrt{2m(E-V)}}{\hbar}$

$R_{reflected} = \left| \frac{J_{reflected}}{J_{incident}} \right| \Rightarrow \frac{|B|^2}{|A|^2}$, $T = \frac{|J_{transmitted}|}{|J_{incident}|} = \frac{|C|^2}{|A|^2}\frac{k_2}{k_1}$

$J_{inc} = \frac{i\hbar}{2m}\left(\psi_1(x)\frac{d\psi_1^*(x)}{dx} - \psi_1^* \frac{d\psi_1(x)}{dx} \right) = \frac{\hbar k_1}{m}|A|^2$

$\Rightarrow J_{reflected} = -\frac{\hbar k_1}{m}|B|^2$, $J_{tra} = \frac{\hbar k_2}{m}|C|^2$

Boundary condition $\Rightarrow$

$A + B = C$

$(A - B)k_1 = Ck_2$

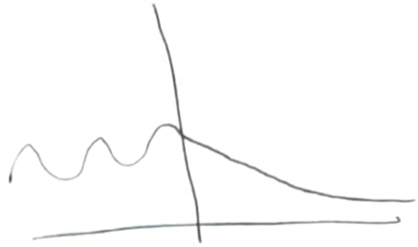
$B = \frac{k_1 - k_2}{k_1 + k_2} A$, $C = \frac{2k_1}{k_1 + k_2} A$ $\Rightarrow$

$R = \frac{(1-K)^2}{(1+K)^2}$, $K = \frac{k_1}{k_2}$, $K = \sqrt{1 - \frac{V_0}{E}}$

$T = \frac{4K}{(1+K)^2} \Rightarrow R + T = 1$

E<V₀

$$\Psi(x,t) = \begin{cases} Ae^{i(k_1 x - \omega t)} + Be^{-i(k_1 x - \omega t)} \\ Ce^{-k_2 x} e^{-i\omega t} \end{cases}$$



$$J(r,t) = \frac{i\hbar}{2m}\left(\Psi \nabla \Psi^* - \Psi^* \nabla \Psi\right)$$

$$\Rightarrow J_T = 0 \quad \left(\Psi_T(x)^2 = \text{real}\right)$$

$J_R = 1$

~~Potential barrier~~

Box potential

proven

$$\Psi_{n_x n_y n_z}(x,y,z) = \sqrt{\frac{8}{abc}} \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{b}\right) \sin\left(\frac{n_z \pi z}{b}\right)$$

$$E_{n_x n_y n_z} \overset{(\text{sum})}{=} \frac{\hbar^2 \pi^2}{2m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$$

(for cubic box)

$$\Rightarrow E_{111} = 3E_1$$ zeropoint energy

(111)

(211) (121) (112)

(221) (212) (122)

(311) (131) (113)

(222)

(321), (312) (213) (231) (132) (123)

Harmonic oscillator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2 \Rightarrow \hat{H} = \frac{\hbar\omega}{2}(\hat{p}^2 + q^2)$$

$$\hat{p} = \frac{\hat{P}}{\sqrt{m\hbar\omega}}, \quad \hat{q} = \hat{x}\sqrt{\frac{m\omega}{\hbar}}$$ /Hermitian Dimentionless op

Harmonic Oscillator Eigenvalue Problem.

Hamitonian of a particle of mass m which oscilates with an angular freqency ω under the influence of a 1D Harmonic potentian. $\frac{1}{2}kx^2$

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \quad -(1) \quad (KE + PE)$$

$[\hat{x}, \hat{p}] = i\hbar$

Algebric methode. (operator methode)

let us define hermitian & Dimention lessopera

$$\hat{p} = \frac{\hat{P}_{momentum}}{\sqrt{m\hbar\omega}}, \quad \hat{q} = \hat{x}\sqrt{\frac{m\omega}{\hbar}} \quad -(2)$$

$$H = \frac{m\hbar\omega\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2\frac{\hbar}{m\omega}$$

$$(1) \Rightarrow \hat{H} = \frac{\hbar\omega}{2}(\hat{p}^2 + \hat{q}^2) \quad -(3)$$

re write hamitonian in terms of hermitian dimentionless operators

let us introduce two more operator which are agian dimentionless

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{q} + i\hat{p}) \qquad \hat{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{q} - i\hat{p}) \quad -(4)$$

~~Let definde Commutator with~~ $a \,\&\, a^\dagger$

$$\hat{a}\hat{a}^\dagger = \frac{1}{2}(\hat{q} - i\hat{p})(\hat{q} + i\hat{p}) = \frac{1}{2}(\hat{q}^2 + \hat{p}^2 + i\hat{q}\hat{p} - i\hat{p}\hat{q})$$

$$= \frac{1}{2}(\hat{q}^2 + \hat{p}^2) + \frac{i}{2}[\hat{q}, \hat{p}] \quad -(5)$$

$$[\hat{q}, \hat{p}] = \left[\sqrt{\frac{m\omega}{\hbar}}\hat{x}, \frac{1}{\sqrt{\hbar m\omega}}\hat{p}\right]$$

$$= \sqrt{\frac{m\omega}{\hbar^2 m\omega}}\hat{x}\hat{p} - \sqrt{\frac{m\omega}{\hbar^2 m\omega}}\hat{p}\hat{x} = \frac{1}{\hbar}[\hat{x}\hat{p} - \hat{p}\hat{x}]$$

$$[\hat{q},\hat{p}] = \frac{1}{\hbar}[\hat{x},\hat{p}] = \frac{i\hbar}{\hbar} = i \quad -(6)$$

$$\Rightarrow \hat{a}^{+}a = \frac{1}{2}(\hat{q}^2+\hat{p}^2) - \frac{1}{2} \quad \text{or}$$

$$\frac{1}{2}(\hat{q}^2+\hat{p}^2) = \hat{a}^{+}\hat{a} + \frac{1}{2} \quad -(7)$$

(3) $\Rightarrow \hat{H} = \hbar\omega\left(\hat{a}^{+}\hat{a}+\frac{1}{2}\right)$, let $\boxed{\hat{a}^{+}\hat{a} = \hat{N}}$, Number operator, which Hermitian

$$\Rightarrow \boxed{\hat{H} = \hbar\omega\left(\hat{N}+\frac{1}{2}\right)} \Rightarrow (9)$$

Define commutator $\hat{a}$ with $\hat{a}^{+}$ $\quad \frac{AB-BA}{\sqrt{2}\sqrt{2}}$

taken out $\frac{1}{\sqrt{2}\sqrt{2}}$

$$[\hat{a},\hat{a}^{+}] = \frac{1}{2}[\hat{q}+i\hat{p}, \hat{q}-i\hat{p}] \Rightarrow (\hat{q}^2+\hat{p}^2-2\hat{q}i\hat{p}) - (\hat{q}^2+p^2-2i\hat{p}\hat{q})$$

$$= \frac{2}{2}i(\hat{p}\hat{q}-\hat{q}\hat{p}) = i[\hat{p},\hat{q}]$$

$$= -i[\hat{q},\hat{p}] = -i \times i = \boxed{1 = [\hat{a},\hat{a}^{+}]} \quad (10) \neq \hat{N}$$

$$[\hat{a}^{+},\hat{a}] = -1$$

Commuta.

$$[\hat{H},\hat{N}] = 0 \quad \hbar\omega\left[\hat{N}+\frac{1}{2}, \hat{N}\right] = 0$$

Thus $\hat{H}$ commute with $\hat{N}$ therefor two operator can have ~~point~~ joint eigen state. $|n\rangle$

Let us assume that joint eigen state is $|n\rangle$

$\hat{N}|n\rangle = n|n\rangle$ — (11) $|n\rangle$ eigenstate

$\hat{H}|n\rangle = E_n|n\rangle$ — (12) n eigen value,

(9) & (12) ⇒

$\hat{H} = \hbar\omega(\hat{N} + \frac{1}{2})$ — (9)

$E_n |n\rangle = \hbar\omega(n + \frac{1}{2})|n\rangle$

$$E_n = (n + \tfrac{1}{2})\hbar\omega$$

physical meaning of $\hat{a}$ & $\hat{a}^+$ operator.

(9) $\hat{H} = \hbar\omega(\hat{N} + \frac{1}{2})$, $\hat{N} = \hat{a}^+\hat{a}$

$[\hat{a}^+\hat{a}] = 1$ — (10)

$[\hat{a}, \hat{H}] = \hbar\omega[\hat{a}, \hat{N} + \frac{1}{2}]$

$[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$

$[\hat{a}, \hat{N}] = [\hat{a}, \hat{a}^+\hat{a}] = [\hat{a}, \hat{a}^+]\hat{a} + \hat{a}^+\underbrace{[\hat{a}, \hat{a}]}_{0} = \hat{a}$

$\because [\hat{a}^+, \hat{a}^+] = 0$

$[\hat{A}, \hat{B} + C] = [\hat{A}, \hat{B}]$ just expand

$[\hat{a}, \hat{H}] = \hbar\omega\hat{a}$

similarly $[\hat{a}^+, \hat{N}] = [\hat{a}^+, \hat{a}^+\hat{a}] = \hat{a}^+[\hat{a}^+, \hat{a}] = -\hat{a}^+$

$[\hat{a}^+, \hat{H}] = -\hbar\omega\hat{a}^+$

Equation (12) ⇒ $\hat{H}|n\rangle = E_n|n\rangle$ inserting $\hat{a}$

$\hat{H}(\hat{a}|n\rangle) = (\hat{a}\hat{H} - \hbar\omega\hat{a})|n\rangle$

$[\hat{a}, \hat{H}] = \hat{a}\hat{H} - \hat{H}\hat{a} = \hbar\omega\hat{a}$

$\hat{H}\hat{a} = \hat{a}\hat{H} - \hbar\omega\hat{a}$

$E_n|n\rangle - \hbar\omega\hat{a}|n\rangle = (E_n - \hbar\omega)(\hat{a}|n\rangle)$ — (17)

$$\hat{H}(\hat{a}^\dagger|n\rangle) = (\hat{a}^\dagger \hat{H} + \hbar\omega \hat{a}^\dagger)|n\rangle = (E_n + \hbar\omega)(\hat{a}^\dagger|n\rangle) \quad \text{--- (18)}$$

$[\hat{a}^\dagger, \hat{H}] \Rightarrow \hat{a}^\dagger \hat{H} - \hat{H}\hat{a}^\dagger = -\hbar\omega \hat{a}^\dagger$

$(\hat{a}^\dagger E_n|n\rangle + \hbar\omega \hat{a}^\dagger|n\rangle)$

from eqn (17) & (18)

$\Rightarrow \hat{a}|n\rangle$ and $\hat{a}^\dagger|n\rangle$ these are the eigenstates of $\hat{H}$ with eigen values $(E_n - \hbar\omega)$ & $(E_n + \hbar\omega)$ respectively

action of $\hat{a}$ & $\hat{a}^\dagger$ will produce new Eigenstates lower and higher by units of $\hbar\omega$

$\hat{a} \rightarrow$ lowering operator ; $\hat{a}^\dagger$ - raising operator.

creation operator

~~Anihilation~~ &

Annihilation and ~~creation~~ or (ladder operator) $\pm\hbar\omega$

How operator $\hat{a}$ and $\hat{a}^\dagger$ act on energy Eigen state $|n\rangle$

Eqn (11) $\Rightarrow \hat{N}|n\rangle = n|n\rangle$ | $[\hat{N}, \hat{a}] = -\hat{a}$, $\hat{N} = \hat{a}^\dagger\hat{a}$

$$[\hat{a}^\dagger\hat{a}, \hat{a}] = \hat{a}^\dagger\underbrace{[\hat{a}, \hat{a}]}_{0} + \hat{a}[\hat{a}^\dagger, \hat{a}] = \hat{a} \times -1 =$$

$$[\hat{N}, \hat{a}] = \hat{N}\hat{a} - \hat{a}\hat{N} = -\hat{a} \Rightarrow \hat{N}\hat{a} = \hat{a}(\hat{N} - 1) \Leftarrow \text{(19.a)}$$

(19)

$$[\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger = \hat{N}\hat{a}^\dagger - \hat{a}^\dagger\hat{N}$$

Similarly

$$[\hat{a}^\dagger\hat{a}, \hat{a}^\dagger] \Rightarrow \hat{a}^\dagger\underbrace{[\hat{a}, \hat{a}^\dagger]}_{1} + 0 \Rightarrow \hat{N}\hat{a}^\dagger = \hat{a}^\dagger(\hat{N} + 1) \Leftarrow \text{(19.b)}$$

$(E_n+\hbar\omega)(\hat a^\dagger|n\rangle)$ — (18)

$n\rangle)$

eigenstates of

$(E_n-\hbar\omega)$ &

$(E_n+\hbar\omega)$ respectiv

e new Eigenstates

ising operator.

ation opera

$\pm\hbar\omega$

state $|n\rangle$

, $N=\hat a^\dagger\hat a$

$x-1=$ } 19

$1) \Leftarrow$ (19.a)

$=\hat N\hat a^\dagger-\hat a^\dagger\hat N$

$\hat N\hat a^\dagger=\hat a^\dagger(\hat N+1)$ $\Leftarrow$ (19.b)

$$\hat N(\hat a|n\rangle) = \underbrace{\hat a(\hat N-1)}_{(19.a)}|n\rangle = (n-1)(\hat a|n\rangle) \quad — (20)$$

$$\hat N(\hat a^\dagger|n\rangle) = \underbrace{\hat a^\dagger(\hat N+1)}_{(19.b)}(\hat a^\dagger|n\rangle) = (n+1)(\hat a^\dagger|n\rangle) \quad — (21)$$

$\Rightarrow$ $\hat a|n\rangle$ & $\hat a^\dagger|n\rangle$ are the Eigenstate of number operator $\hat N$ with eigen value $(n-1)$ & $(n+1)$ ~~effectively~~ respectively.

$\hat a$ & $\hat a^\dagger$ will decrese & increse the value of N by one unit. (The action of $\hat a$ on $|n\rangle$ generate new state $|n-1\rangle$ ie $\hat a|n\rangle \sim |n-1\rangle$)

~~when~~

$\Rightarrow \hat a|n\rangle \Rightarrow C_n|n-1\rangle$ — (22)

$\hat a^\dagger|n\rangle \Rightarrow C_n|n+1\rangle$, — (23)

} C_n has to be determined (from Normalization of ...)

Normalization $\Rightarrow (\hat a|n\rangle)^\dagger(\hat a|n\rangle)$

(22) $\Rightarrow$ ~~$(\hat a|n\rangle)$~~ $\times\,(\langle n|\hat a^\dagger).(\hat a|n\rangle) \Rightarrow \langle n|\hat a^\dagger).C_n|n-1\rangle$

$\langle n|\hat a^\dagger\hat a|n\rangle = C_n\langle n|\hat a^\dagger|n-1\rangle$ $\xrightarrow{(23)}$ $\langle n|C_n|n\rangle$

$= C_nC_n\langle n|n\rangle$

$\langle n|\hat a^\dagger\hat a|n\rangle = C_n^2$ — (24)

(11) $\Rightarrow \hat N|n\rangle = n|n\rangle$

$\langle n|\hat N|n\rangle = n\langle n|n\rangle$ — (25)

$\langle n|\hat a^\dagger\hat a|n\rangle = n$

(24) $\Rightarrow C_n^2 = n$

$C_n = \sqrt n$

(22) ⟹ $\boxed{\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle}$ 26 — n has to be ...

Similary,

$$\boxed{\hat{a}^{+}|n\rangle = \sqrt{n+1}\,|n+1\rangle}$$

└ increases the Eigen ... by one unit

(23) ⟹ Normalization

$$\langle n|\hat{a}\hat{a}^{+}|n\rangle = \langle n|\hat{a}\, C_n|n+1\rangle$$

$$= C_n\langle n|\hat{a}|n+1\rangle$$

$$\langle n|\hat{a}\hat{a}^{+}|n\rangle = C_n^2\langle n|n\rangle = C_n^2 \longrightarrow$$

(25) ⟹ $\langle n|\hat{a}^{+}\hat{a}|n\rangle = n$ | $[\hat{a},\hat{a}^{+}] = \hat{a}\hat{a}^{+} - \hat{a}^{+}\hat{a} = 1$

$$\langle n|\hat{a}\hat{a}^{+} - 1|n\rangle = n$$

$$\langle n|\hat{a}^{+}\hat{a}|n\rangle - 1\langle n|n\rangle = n \quad \Rightarrow C_n^2 = n+1$$

$$\langle n|\hat{a}^{+}\hat{a}|n\rangle = n+1 \longrightarrow C_n = \sqrt{n+1}$$

Energy Eigen States

($\hat{a}$ & $\hat{a}^{+}$ decreases or increase energy Eigen value)

zero state (groundstate)

$\hat{a}^{+}|0\rangle = |1\rangle$ or $|1\rangle = \hat{a}^{+}|0\rangle$ —(1) $\hat{a}^{+}|n\rangle = \sqrt{n+1}\,|n+1\rangle$

~~Grou~~ first state = operating $\hat{a}^{+}$ on groundstate.

$$|2\rangle = \frac{1}{\sqrt{2}}\hat{a}^{+}|1\rangle = \frac{1}{\sqrt{2!}}(\hat{a}^{+})^2|0\rangle \quad -(2)$$

$$|3\rangle = \frac{1}{\sqrt{3}} \hat{a}^{+} |2\rangle = \frac{1}{\sqrt{3!}} (\hat{a}^{+})^3 |0\rangle \quad - (3)$$

eigen vectors in terms of ground state

$$|n\rangle = \frac{1}{\sqrt{n}} \hat{a}^{+} |n-1\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^{+})^n |0\rangle$$

$\hat{a} |n-1\rangle = \sqrt{n} |n\rangle$

$$\hat{a}^{+} |n\rangle = \sqrt{n+1}\, |n+1\rangle$$

$$\hat{a}^{+} |1\rangle = \sqrt{2}\, |2\rangle$$

$$|2\rangle = \frac{1}{\sqrt{2}} \hat{a}^{+} |1\rangle$$

Enegy Eigen States In position ~~states~~ Space.

determine harmonic oscilator wavefunction (ψ) in Position rep. find determine ground state ψ in position then use $\hat{a}^{+}$ to find next

$$\hat{p} = \frac{\hat{P}}{\sqrt{m\hbar\omega}} \; ; \quad \hat{q} = \hat{x} \sqrt{\frac{m\omega}{\hbar}}$$

$\Rightarrow \hat{p}$ in position space.

$$\hat{p} = \frac{-i\hbar}{\sqrt{m\hbar\omega}} \frac{d}{dx} = -i x_0 \frac{d}{dx} \; , \quad x_0 = \sqrt{\frac{\hbar}{m\omega}}$$

= Constant & have dimentions length.

$$\hat{q} = \frac{\hat{x}}{x_0}$$

$\Rightarrow a \,\&\, a^{+}$ in Position Space.

$$\Rightarrow \hat{a} = \frac{1}{\sqrt{2}} (\hat{q} + i\hat{p}) = \frac{1}{\sqrt{2}} \left(\frac{\hat{x}}{x_0} + i x - i x_0 \frac{d}{dx} \right)$$

$$= \frac{1}{\sqrt{2}} \left(\frac{\hat{x}}{x_0} + x_0 \frac{d}{dx} \right) = \frac{1}{\sqrt{2}\, x_0} \left(\hat{x} + x_0^2 \frac{d}{dx} \right) \quad - (3)$$

$$\hat{a}^{+} = \frac{1}{\sqrt{2}} (\hat{q} - i\hat{p}) = \frac{1}{\sqrt{2}} \left(\frac{x}{x_0} - x_0 \frac{d}{dx} \right) = \frac{1}{\sqrt{2}\, x_0} \left(\hat{x} - x_0^2 \frac{d}{dx} \right) \quad (4)$$

$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle$

$\hat{a}|0\rangle = 0$ — ④ ③

$\langle x|\hat{a}|0\rangle = \frac{1}{\sqrt{2}\,x_0}\langle x|\hat{x} + x_0^2 \frac{d}{dx}|0\rangle = 0$ $\qquad \psi_n(x) = \langle x|n\rangle$

$= \frac{1}{\sqrt{2}\,x_0}\left(x\,\psi_0(x) + x_0^2 \frac{d\psi_0(x)}{dx}\right) = 0$, $\quad \psi_0(x) = \langle x|0\rangle$ (ground wave fn)

$\Rightarrow \frac{d\psi_0(x)}{dx} = -\frac{x}{x_0^2}\,\psi_0(x)$ — ⑤

$\int \frac{1}{\psi_0(x)}\,d\psi_0(x) = -\frac{1}{x_0^2}\int x\,dx$

$\log\psi_0(x) = -\frac{1}{x_0^2}\cdot\frac{x^2}{2} + \log A$

$\Rightarrow \boxed{\psi_0(x) = A\exp\left[\frac{-x^2}{2x_0^2}\right]}$ — ⑥ GS wavefunction of harmonic oscillator.

A can be find out by Normalization Condition.

$\int_{-\infty}^{\infty} |\psi_0(x)|^2\,dx = 1$

$A^2 \int_{-\infty}^{\infty} \exp\left[\frac{2x^2}{2x_0^2}\right] = 1$

$\because \int_{-\infty}^{\infty} e^{-x^2/a}\,dx = \sqrt{\pi}\sqrt{a}$ gaussian integral.

$\Rightarrow A^2\sqrt{\pi}\,x_0 = 1 \quad \Rightarrow A = \frac{1}{\sqrt{\sqrt{\pi}\,x_0}}$, $x_0 = \sqrt{\frac{\hbar}{m\omega}} \Rightarrow A = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$

$$\Rightarrow \boxed{\psi_0(x) = \frac{1}{\sqrt{\sqrt{\pi}\, x_0}} \exp\left(-\frac{x^2}{2x_0^2}\right)}$$

— Solution of Harmonic oscillator
→ Gaussian function
→ Ground state

$\langle x|0\rangle$

First exited state.

$$\langle x|1\rangle = ? = \langle x|\hat{a}^{+}|0\rangle$$

$\psi_1(x)$

$$= \frac{1}{\sqrt{2}x_0}\left(x - x_0^2 \frac{d}{dx}\right)\langle x|0\rangle \quad \psi_0(x)$$

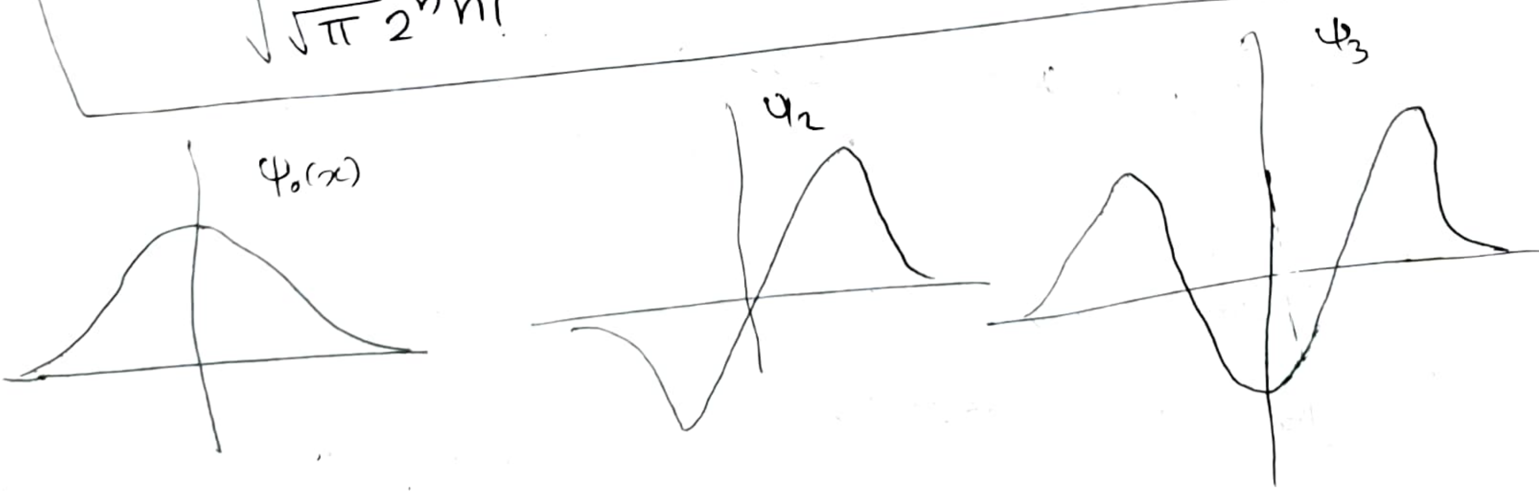
$$= \frac{1}{\sqrt{2}x}\left(x - x_0^2\left(-\frac{x}{x_0^2}\right)\right)\psi_0(x) = \frac{\sqrt{2}}{x_0} x\,\psi_0(x)$$

$$\psi_1(x) = \frac{\sqrt{2}}{x_0} x\,\psi_0(x) = \sqrt{\frac{2}{\sqrt{\pi}\, x_0^3}}\; e\left(\frac{-x^2}{2x_0^2}\right) \quad (8)$$

Similarly $\langle x|2\rangle = \psi_2$ ⇒ General

$\langle x|3\rangle = \psi_3$

$$\boxed{\psi_n(x) = \frac{1}{\sqrt{\sqrt{\pi}\, 2^n n!}} \frac{1}{x_0^{n+1/2}} \left(x - x_0^2 \frac{d}{dx}\right)^n e^{-x^2/2x_0^2}}$$



As for the eigen state of second and third exited state, we can obtain them by appling $\hat{a}^+$ on the ground state twise and thrice time respectiely

$$\langle x|2\rangle = \frac{1}{\sqrt{2!}} \langle x|(a^+)^2|0\rangle = \frac{1}{\sqrt{2!}}\left(\frac{1}{\sqrt{2}\,x_0}\right)^2\left(x - x_0^2\frac{d}{dx}\right)^2 \psi_0(x)$$

~~$\psi_2(x)$~~ =

$$\langle x|3\rangle = \frac{1}{\sqrt{3!}} \langle x|(a^+)^3|0\rangle = \frac{1}{\sqrt{3!}}\left(\frac{1}{\sqrt{2}\,x_0}\right)^3\left(x - x_0^2\frac{d}{dx}\right)^3 \psi_0 x$$

Similar

$$\langle x|n\rangle = \frac{1}{\sqrt{n!}} \langle x|(a^+)^n|0\rangle = \frac{1}{\sqrt{n!}}\left(\frac{1}{\sqrt{2}x_0}\right)^n\left(x - x_0^2\frac{d}{dx}\right)^n \psi_0(x)$$

Matrix representation of operator in $\{|n\rangle\}$

$\hat{a}, \hat{a}^+, \hat{x}, \hat{P}, \hat{N}, \hat{H}$ — Number op

—

$\hat{N}|n\rangle = n|n\rangle$

$\hat{H}|n\rangle = E_n|n\rangle$

} , $E_n = (n+\frac{1}{2})\hbar\omega$ — $\hat{H}$ & $\hat{N}$ are represented by same Eigen state.

also $[\hat{H}, \hat{N}] = 0$, Commute

Have common eigenstate.

To find matrix element

$\hat{N}|n\rangle = n|n\rangle$

$\langle n'|\hat{N}|n\rangle = n\langle n'|n\rangle$ — $|n\rangle$ & $|n'\rangle$ are orthonormal

$= n\,\delta_{n'n}$ ① Finite when $n' = n$

$\langle n'|\hat{H}|n\rangle = \hbar\omega\left(n+\frac{1}{2}\right)\delta_{n'n}$ — (2)

$$\begin{bmatrix} 00 & 01 & 02 & \cdots \\ 10 & 11 & \cdots & \\ 20 & \cdots & & \\ \vdots & & & \end{bmatrix}$$

* General any operator $[\hat{n}]$

$n' = n$ ⇒ Diagonal elements

for $\hat{N} = \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 2 & 0 & \cdots \\ & & & 3 & \\ \vdots & & & & \ddots \end{bmatrix}$

$$\hat{H} = \frac{\hbar\omega}{2}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ \vdots & & & \ddots \end{bmatrix}$$

n = 0
n = 1
n = 2

$[\hat{a}, N] \neq 0$ & $[\hat{a}^{\dagger}, N] \neq 0$ ⇒ no diagonal

Similarly

$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle$

for element

$\langle n'|\hat{a}|n\rangle = \sqrt{n}\,\delta_{n'(n-1)}$

in general

$$\hat{a} = \begin{bmatrix} 00 & 01 & 02 & \cdots \\ 10 & 11 & 12 & \cdots \\ 20 & 21 & 22 & \cdots \\ \vdots & & & \ddots \end{bmatrix}$$

$\hat{a}^{\dagger}|n\rangle = \sqrt{n+1}\,|n+1\rangle$

$\langle n'|\hat{a}^{\dagger}|n\rangle = \sqrt{n+1}\,\delta_{n'(n+1)}$

$n' = (n-1)$ ⇒ ~~diagonal~~ only fine in area above diagonal

$$\hat{a} = \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & & & & & \ddots \end{bmatrix}$$

Similarly $\qquad (n' = n+1)$

$$a^{+} = \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & & & & \ddots \end{bmatrix}$$

$\hat{x} =$

We already know $\hat{a}$ & $\hat{a}^{+}$ matrix form, so in terms of $\hat{a}$ & $\hat{a}^{+}$

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{q} + i\hat{p})$$

$$\hat{a}^{+} = \frac{1}{\sqrt{2}}(\hat{q} - i\hat{p})$$

$$\hat{q} = \hat{x}\sqrt{\frac{m\omega}{\hbar}}$$

$$\hat{p} = \frac{\hat{p}}{\sqrt{m\hbar\omega}}$$

$\hat{x}$ in $\hat{a}$ & $\hat{a}^{+}$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^{+})$$

$$\hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^{+} - \hat{a})$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & & & & \end{bmatrix}$$

$\Rightarrow \langle n|\hat{x}|n\rangle = 0$

$\langle n|\hat{p}|n\rangle = 0$

$$\hat{p} = i\sqrt{\frac{m\hbar\omega}{2}} \begin{bmatrix} 0 & \sqrt{1} & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & & & & \end{bmatrix}$$

$\hat{p}^\dagger = \hat{p}$ but $\hat{p}^* = -\hat{p}$ hermitian

$\hat{x}^\dagger = \hat{x}$ & $\hat{x}^* = \hat{x}$ hermitian & complex conjugate sa..

Eigen vectors matrix rep

$|n\rangle$ = coulmn

$|0\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \end{bmatrix}$, $|1\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \end{bmatrix}$, $|2\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{bmatrix}$

Expectation values of various operators ($\hat{x}^2$ & $\hat{p}^2$)

$x = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger)$; $\hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^\dagger - \hat{a})$

$[a, \hat{a}^\dagger] = 1$

$\hat{x}^2 = \frac{\hbar}{2m\omega}(\hat{a}^2 + \hat{a}^{\dagger 2} + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}) = \frac{\hbar}{2m\omega}(\hat{a}^2 + \hat{a}^{\dagger 2} + \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a})$

add and subtract

$\hat{x}^2 = \frac{\hbar}{2m\omega}(\hat{a}^2 + \hat{a}^{\dagger 2} + 2\hat{a}^\dagger\hat{a} + 1)$ — ①

$\hat{p}^2 = \frac{-m\hbar\omega}{2}(\hat{a}^2 + \hat{a}^{\dagger} - \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a})$ ~~$= \frac{m\hbar\omega}{}$~~ $(-1 + \hat{a}\hat{a}^\dagger - \hat{a}\hat{a}^\dagger$ -1

$= \frac{m\hbar\omega}{2}(\hat{a}^2 + \hat{a}^{\dagger 2} - 2\hat{a}^\dagger\hat{a} - 1)$ — ②

$\langle n|\hat{a}^2|n\rangle - \langle n|\hat{a}^{\dagger 2}|n\rangle = 0$, expectation value

$\langle n|\hat{a}^\dagger\hat{a}|n\rangle = \langle n|\hat{N}|n\rangle = n$

① $\Rightarrow \langle n|\hat{x}^2|n\rangle = \frac{\hbar}{2m\omega}(2n+1) = \frac{1}{m\omega^2}\left[\left(n+\frac{1}{2}\right)\hbar\omega\right]$ — ③

② $\Rightarrow \langle n|\hat{p}^2|n\rangle = -\frac{m\hbar\omega}{2}(-2n-1) = m\left[\left(n+\frac{1}{2}\right)\hbar\omega\right]$ — ④

③ $\Rightarrow \frac{1}{2}m\omega^2\langle n|\hat{x}^2|n\rangle = \frac{1}{2}(n+1/2)\hbar\omega$ — ⑤ ($\times \frac{1}{2}$ both side) - PE

④ $\Rightarrow \frac{1}{2m}\langle n|\hat{p}^2|n\rangle = \frac{1}{2}(n+1/2)\hbar\omega$ — ⑥ ($\times \frac{1}{2}$ both side) - KE

$\frac{1}{2}m\omega^2\langle n|$

Expectation (or avarage) value of KE & PE are equal and are also equals to half of total expectation value energy $[(n+1/2)\hbar\omega]$ expectation value of Hamiltonian

$$\Rightarrow \frac{m\omega^2}{2}\langle n|\hat{x}^2|n\rangle = \frac{1}{2m}\langle n|\hat{p}^2|n\rangle = \frac{1}{2}\langle n|H|n\rangle$$

Virial theorm

Expectation value of squre of position and momentum operator is equals to half of the total Energy

Isotropic harmonic oscillator potential

$\omega_x = \omega_y = \omega_z = \omega$

$$\hat{V}(x,y,z) = \frac{1}{2}m\omega^2\hat{x}^2 + \frac{1}{2}m\omega^2\hat{y}^2 + \frac{1}{2}m\omega^2\hat{z}^2$$

$$E_{n_x n_y n_z} = \left(n_x + n_y + n_z + \frac{3}{2}\right)\hbar\omega \quad \text{in 3D} \quad (1)$$

($\frac{3}{2} = \frac{1}{2} + \frac{1}{2} + \frac{1}{2}$)

For ground state $n_x = n_y = n_z = 0$

$$E_{000} = \frac{3\hbar\omega}{2}$$

Degeneracy

$$g_n = \frac{1}{2}(n+1)(n+2) \quad (2)$$

where $n = n_x + n_y + n_z$

⇒ First exited state. $(n=1)$

$g_1 = 3$

Possible combinations (100), (010), (001) } 3 fold degenerate.

$$E_{100} = E_{001} = E_{010} = \frac{5}{2}\hbar\omega$$

⇒ second exited state.

$n=2$, $g_2 = \frac{1}{2}(n+1)(n+2) = \frac{1}{2}(2+1)\cdot(2+2) = 6$

6 fold degenerate.

(200), (020), (002), (110), (101), (011)

$$E_{200} = E_{002} = E_{020} = E_{110} = E_{101} = E_{011} = \frac{7}{2}\hbar\omega$$

⇒ 3rd Exited State

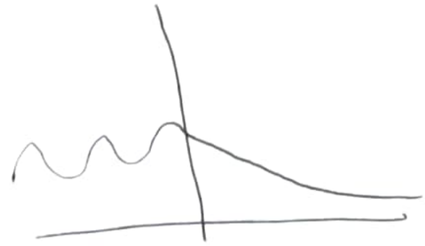
$n=3$, $g_3 = \frac{1}{2}(3+1)(3+2) = 10$

(300), (030), (003), (210), (201), (021), (120), (111), (102), (012)

$E_3 = 9/2\,\hbar\omega$

E<v₀

$$\psi(x,t) = \begin{cases} Ae^{i(k_1x-\omega t)} + Be^{-i(k_1x-\omega t)} \\ Ce^{-k_2 x}e^{-i\omega t} \end{cases}$$



$$J(r,t) = \frac{i\hbar}{2m}\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right)$$

$\Rightarrow J_T = 0$ $\left(\psi_T(x)\ \text{real}\right)$

$J_R = 1$

~~Potential barrier~~

Box Potention / proof

$$\psi_{n_x n_y n_z}(x,y,z) = \sqrt{\frac{8}{abc}}\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{b}\right)\sin\left(\frac{n_z\pi z}{b}\right)$$

$$E_{n_x n_y n_z} \overset{(\text{Sum})}{=} \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$$

$\Rightarrow E_{111} = 3E_1$ (for cubic box)

zeropoint energy

(111)

(211) (121) (112)

(221) (212) (122)

(311) (131) (113)

(222)

(321), (312) (213) (231) (132) (123)

Harmonic oscillator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \Rightarrow \hat{H} = \frac{\hbar\omega}{2}\left(\hat{p}^2 + q^2\right)$$

$$\hat{p} = \frac{\hat{P}}{\sqrt{m\hbar\omega}},\quad \hat{q} = \hat{x}\sqrt{\frac{m\omega}{\hbar}}$$ / Hermitian Dimentionless op

$\hat{a} = \frac{1}{\sqrt{2}}(\hat{q} + i\hat{p})$, $\hat{a}^{+}$

$\hat{N}|n\rangle = n|n\rangle$ & $\hat{H}|n\rangle = E_n|n\rangle$

$[q, p] = i$

$\Rightarrow [\hat{H}, \hat{N}] = 0 \Rightarrow$

$\hat{H} = \hbar\omega(\hat{N} + \frac{1}{2})$, $\hat{N} = \hat{a}^{+}\hat{a}$, number op. $E_n = (n + \frac{1}{2})\hbar\omega$

$[\hat{a}, \hat{a}^{+}] = 1$

$[\hat{a}, \hat{H}] = \hbar\omega\hat{a}$

$[\hat{a}^{+}, \hat{H}] = -\hbar\omega\hat{a}^{+}$

$[\hat{N}, \hat{a}] = -\hat{a}$, $[\hat{N}, \hat{a}^{+}] = \hat{a}^{+}$

$\hat{N}(\hat{a}|n\rangle) = (n-1)\hat{a}|n\rangle$

$\hat{a}^{+}|\ \rangle = (\ +\ )\ \hat{a}^{+}\ \rangle$

$\hat{H}(\hat{a}|n\rangle) = (E_n - \hbar\omega)(\hat{a}|n\rangle)$

$a^{+}|\ \rangle = E_n +\ \ |\hat{a}^{+}\rangle$

action on $|n\rangle$

$\hat{a}|n\rangle = c_n|n-1\rangle$

$\hat{a}^{+}|n\rangle = c_n|n+1\rangle$

normalization $\Rightarrow c_n = ?$ $c_n^2 = n$ $c_n = \sqrt{n}$

$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$ & $\hat{a}^{+}|n\rangle = \sqrt{n+1}|n+1\rangle$

$|n\rangle = \frac{1}{\sqrt{n}}\hat{a}^{+}|n-1\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^{+})^{n}|0\rangle$

To determine ψ

$\hat{p} = -i x_0 \frac{d}{dx}$, $x_0 = \sqrt{\frac{\hbar}{m\omega}}$

$q = \frac{\hat{x}}{x_0}$ $\Rightarrow \hat{a} = \frac{1}{\sqrt{2}\,x_0}\left(\hat{x} + x_0^2\frac{d}{dx}\right)$

$\hat{a}^{+}$ ($-$)

$\psi_0 = A\exp\left[\frac{-x^2}{2x_0}\right]$, $A = \frac{1}{\sqrt{\sqrt{\pi}\,x_0}}$

$\psi_n(x) = \frac{1}{\sqrt{\sqrt{\pi}\,2^n n!}} \frac{1}{x_0^{n+1/2}}\left(x - x_0^2\frac{d}{dx}\right)^n e^{-x^2/2x_0^2}$

Matrix representation of operator.

$\hat{N}|n\rangle = n|n\rangle \Rightarrow \langle n'|\hat{N}|n\rangle = n\langle n'|n\rangle = n\,\delta_{n'n}$

$$\hat{N} = \begin{bmatrix} 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 2 & \\ & \vdots & & \end{bmatrix}, \quad \langle n'|\hat{H}|n\rangle = \hbar\omega(n+\tfrac{1}{2})\,\delta_{n'n}$$

$$\hat{H} \Rightarrow \frac{\hbar\omega}{2}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 3 & 0 & \cdots \\ 0 & 0 & 5 & \cdots \\ & \vdots & & \end{bmatrix}$$

$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \Rightarrow \langle n'|\hat{a}|n\rangle = \sqrt{n}\,\delta_{n',(n-1)}$

$$\Rightarrow \hat{a} = \begin{bmatrix} 0 & \sqrt{1} & 0 & \cdots \\ 0 & 0 & \sqrt{2} & \cdots \\ 0 & 0 & 0 & \sqrt{3} \; \cdots \\ \vdots & & \ddots & \end{bmatrix}; \quad \hat{a}^{+} = \begin{bmatrix} 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & \\ 0 & \sqrt{2} & 0 & \cdots \\ \vdots & & \sqrt{2} & \end{bmatrix}$$

$\hat{a} = \frac{1}{\sqrt{2}}(\hat{q} + i\hat{p})$ & $\hat{q} = \hat{x}\sqrt{\frac{m\omega}{\hbar}} \Rightarrow \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^{+})$

$\hat{a}^{+} = \frac{1}{\sqrt{2}}(\hat{q} - i\hat{p})$ $\quad \hat{p} = \frac{\hat{P}}{\sqrt{m\omega\hbar}}$ $\quad \hat{P} = i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^{+} - \hat{a})$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 \\ \sqrt{1} & 0 & \sqrt{2} & \cdots \\ 0 & \sqrt{2} & 0 & \\ & \vdots & & \end{pmatrix}; \quad \hat{P} = i\sqrt{\frac{m\hbar\omega}{2}}\begin{bmatrix} 0 & -\sqrt{1} & & \\ \sqrt{1} & 0 & -\sqrt{2} & \\ \vdots & \sqrt{2} & & \cdots \\ \vdots & & & \end{bmatrix}$$

$$|1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$\frac{m\omega^2}{2}\langle n|\hat{x}^2|n\rangle = \frac{1}{2m}\langle n|\hat{P}^2|n\rangle = \frac{1}{2}\langle n|H|n\rangle$

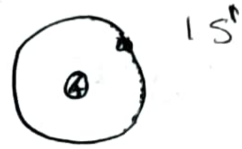
Isotropic harmonic oscilator poten

$E_{n_x n_y n_z} = (n_x + n_y + n_z + \frac{3}{2})\hbar\omega$

degeneracy $g_n = \frac{1}{2}(n+1)(n+2)$, $n = n_x + n_y + n_z$

Hydrogen Atom

Shrödinger equation of Hydrogen atom



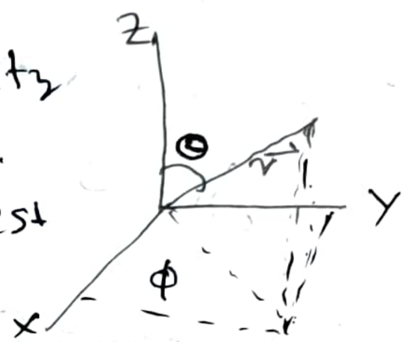
Cartesian form of Shrödinger eqn in 3D

$$U = \frac{-e^2}{4\pi\varepsilon_0 r}$$

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E-U)\psi = 0$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2m}{\hbar^2}(E-U)\psi = 0 \quad -①$$

In SPC Due to spherical Symmetry of the physical Situation. description in spc is the best choice.



$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} + \frac{2m}{\hbar^2}(E-U)\psi = 0 \quad -②$$

$x = r\sin\theta\cos\phi$

$y = r\sin\theta\sin\phi$

$z = r\cos\theta$

↓ U

② × $r^2\sin^2\theta$ ⟹

$$② \Rightarrow \sin^2\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{\partial^2\psi}{\partial\phi} + \frac{2m r^2\sin^2\theta}{\hbar}\left(\frac{e^2}{4\pi\varepsilon_0 r} + E\right)\psi = 0 \quad -③$$

Seperation of variables.

Assume that $\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$ - (4)

$$\frac{\partial \psi}{\partial r} = \Theta\Phi \frac{dR}{dr} ; \quad \frac{\partial \psi}{\partial \theta} = R\Phi \frac{d\Theta}{d\theta} ; \quad \frac{\partial^2 \psi}{\partial \phi^2} = R\Theta \frac{d^2\Phi}{d\phi^2}$$

(3) $\Rightarrow \sin^2\theta \frac{d}{dr}\left(r^2 \frac{dR}{dr}\right)\Theta\Phi + \sin^2\theta \frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right)R\Phi$

$$+ R\Theta \frac{d^2\Phi}{d\phi^2} + \frac{2mr^2 \sin^2\theta}{\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0 r} + E\right)R\Theta\Phi = 0$$

Rdevide $R\Theta\Phi$

$$\Rightarrow \frac{\sin^2\theta}{R} \frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) + \frac{\sin\theta}{\Theta} \frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) + \frac{1}{\Phi} \frac{d^2\Phi}{d\phi^2}$$

$$+ \frac{2mr^2 \sin^2\theta}{\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0 r} + E\right) = 0$$

fn of ϕ only

re arrange

$$\Rightarrow \frac{\sin^2\theta}{R} \frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) + \frac{\sin\theta}{\Theta} \frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right)$$

$$+ \frac{2mr^2 \sin^2\theta}{\hbar^2}\left[\frac{e^2}{4\pi\varepsilon_0 r} + E\right] = \frac{-1}{\Phi} \frac{d^2\Phi}{d\phi^2} \quad \text{- (5)}$$

This eqn can be correct only If bothside of the eqn are equals to same constat. Since they are fn of different variables

- (6)

$$\frac{-1}{\Phi} \frac{d^2\Phi}{d\phi^2} = m_l^2$$

$$\frac{1}{R} \frac{d}{dR}\left(r^2 \frac{dR}{dR}\right) + \frac{2mr^2}{\hbar^2}\left[\frac{e^2}{4\pi\varepsilon_0 r} + E\right] = \frac{m_l^2}{\sin\theta} - \frac{1}{\Theta \sin\theta} \frac{d}{d\theta}\left[\sin\theta \frac{d\Theta}{d\theta}\right]$$

- (7)

LHS is is f^n of R only & RHS f^n of Θ only

$$\frac{m_l^2}{\sin^2\theta} - \frac{1}{\Theta \sin\theta}\frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) = l(l+1) \quad (8)$$

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2mr^2}{\hbar^2}\left[\frac{e^2}{4\pi\varepsilon_0 r} + E\right] = l(l+1) \quad (9)$$

(6) $\frac{d^2\Phi}{d\phi^2} = -m_l^2\Phi$ it is a ordinary DE

$$\Rightarrow \Phi = Ae^{im_l\phi}$$

Since we are dealing with spherical symmetric potential so a change of ϕ by 2π should give same value.

Azimuthal eq^n

$$\Rightarrow e^{im_l(\phi+2\pi)} = e^{im_l\phi}$$

or

$$\frac{e^{im_l(\phi+2\pi)}}{e^{im_l\phi}} = 1$$

$$e^{im_l 2\pi} = 1 \Rightarrow m_l = 0, \pm 1, \pm 2, \pm 3$$

magnetic Quntum number

(8) → Legendre polynomial
(9) → Languerie polynomial
} To solve

Assignment Find out the solution of R & Θ eq^n

Quantum number

Φ eqn ⇒ m_l → magnetic Quatum number

Θ eqn ⇒ l → orbital Quntum number

R eqn ⇒ n → ~~Orbital~~ Principle Quntum number.

Solution of Radial equation (R)

$E_n \propto \frac{1}{n^2}$, $n = 1, 2, 3, \ldots$ 1 to n

physical significance: ~~electron elerg~~ Electron energy is Quantized

Orbit Quntum ~~qua~~ number (l)

magnitude of electron angular momentum is

$L = \sqrt{l(l+1)}\,\hbar$, $l = 0, 1, 2, 3, \ldots (n-1)$;
$\hat{s}, \hat{p}, \hat{d}, \hat{f}$ 0 to (n-1)

$l=0$; $L = 0\hbar$

$l=1$; $L = \sqrt{2}\hbar$

$l=2$; $L = \sqrt{6}\hbar$

⇒ Angular momentum magnitude is quantized.

magnetic Quntum number (m_l) ($-l$ to l) ⇒ $2l+1$ values

Space Quntization.

Not only magnitude but the direction of the angular momentum is quantized



Magnetic Quantum number (m_l) specify the direction of L, by determining the direction of L in field direction

If we assum that magnetic field direction is paralell to 2 direction then the component of L in this direction is given by

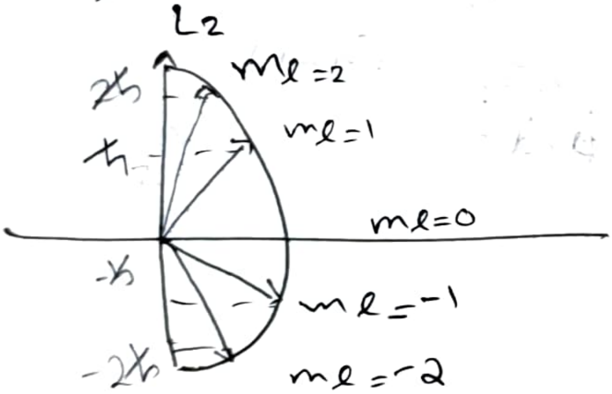
$$L_z = m_l \hbar$$

$m_l = 0, \pm 1, \pm 2, \ldots$

$\Rightarrow 2l+1$ value.

eg: $l = 2$

$m_l = -2, -1, 0, 1, 2$ $\quad L_z = -2\hbar, -\hbar, 0, \hbar, 2\hbar$



H atom

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E-U)\psi = 0 \quad , U = \frac{-e^2}{4\pi\varepsilon_0 r}$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial^2\psi}{\partial\phi^2} + \frac{2m}{\hbar^2}(E-U)\psi = 0$$

$$\frac{m_l^2}{\sin^2\theta} - \frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) = l(l+1)$$

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2mr^2}{\hbar^2}\left[\frac{e^2}{4\pi\varepsilon_0 r} + E\right] = l(l+1)$$

$$\frac{d^2\Phi}{d\phi^2} = m_l\Phi \Rightarrow \Phi = Ae^{im_l\phi} \Rightarrow m_l = 0, \pm1, \pm2 \ldots$$

$$L = \sqrt{l(l+1)}\,\hbar$$

$n = 1, 2 \ldots n$

$l = 0, \ldots (n-1)$ $\quad h_z = m_l\hbar$

$m_l = -l$ to $l \Rightarrow 2l+1$

Angular momentum

$$\vec{L} = \hat{R}\times\hat{P} = -i\hbar\,\hat{R}\times\vec{\nabla}$$

$$[\hat{L}_x, \hat{L}_y] = \hat{L}_z\,\varepsilon_{xyz}\,i\hbar$$

$$[\hat{x}, \hat{L}_y] = \hat{z}\,\varepsilon_{xyz}\,i\hbar$$

$$[P_x, L_y] = P_z\,\varepsilon_{xyz}\,i\hbar$$

$$[c, L_k] = 0 \quad , k = x, y, z$$

Angular momentum

Orbital momentum

$\vec{L} = \vec{r} \times \vec{p} = (y p_z - z p_y)i + (z p_x - x p_z)j + (x p_y - y p_x)k$

QM

$r = \hat{R}$

$\hat{R} = \hat{P} = -i\hbar\vec{\nabla}$

$P_x = -i\hbar \frac{\partial}{\partial x}$

$$\vec{L} = \hat{R} \times \hat{P} = -i\hbar \hat{R} \times \vec{\nabla} \quad -(1)$$

$$L_x = \hat{y}\hat{P}_z - \hat{z}\hat{P}_y = -i\hbar\left(\hat{y}\frac{\partial}{\partial z} - \hat{z}\frac{\partial}{\partial y}\right) \quad -(2)$$

$$L_y = \hat{z}\hat{P}_x - \hat{x}\hat{P}_z = -i\hbar\left(\hat{z}\frac{\partial}{\partial x} - \hat{x}\frac{\partial}{\partial z}\right) \quad -(3)$$

$$L_z = \hat{x}\hat{P}_y - \hat{y}\hat{P}_x = -i\hbar\left(\hat{x}\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \quad -(4)$$

$$L^2 = L_x^2 + L_y^2 + L_z^2 = L_x L_x + L_y L_y + L_z L_z$$

Commutation relations

$[\hat{x}, \hat{y}] = [\hat{y}, \hat{z}] = [\hat{z}, \hat{x}] = 0$

$[P_x, P_y] = [\hat{P}_y, \hat{P}_z] = [\hat{P}_z, \hat{P}_x] = 0$

$[\hat{x}, \hat{P}_x] = i\hbar = [\hat{y}, \hat{P}_y] = [\hat{z}, \hat{P}_z]$

$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$

$[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$

$[\hat{L}_z, \hat{L}_x] = i\hbar L_y$

$[\hat{x}, \hat{L}_x] = 0$

$[x, L_y] = i\hbar \hat{z}$

$[x, L_z] = -i\hbar y$

Angular momentum

orbital momentum

$$\vec{L} = \vec{r} \times \vec{p} = (y p_z - z p_y) i + (z p_x - x p_z) j + (x p_y - y p_x) k$$

QM

$r = \hat{R}$

$\hat{P} = \hat{p} = -i\hbar \vec{\nabla}$

$P_x = -i\hbar \frac{\partial}{\partial x}$

$$\vec{L} = \hat{R} \times \hat{p} = -i\hbar \hat{R} \times \vec{\nabla} \quad -(1)$$

$$L_x = \hat{y} \hat{P}_z - \hat{z} \hat{P}_y = -i\hbar \left(\hat{y} \frac{\partial}{\partial z} - \hat{z} \frac{\partial}{\partial y} \right) \quad -(2)$$

$$L_y = \hat{z} \hat{P}_x - \hat{x} \hat{P}_z = -i\hbar \left(\hat{z} \frac{\partial}{\partial x} - \hat{x} \frac{\partial}{\partial z} \right) \quad -(3)$$

$$L_z = \hat{x} \hat{P}_y - \hat{y} \hat{P}_x = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \quad -(4)$$

$$L^2 = L_x^2 + L_y^2 + L_z^2 = L_x L_x + L_y L_y + L_z L_z$$

Commutation relations

$$[\hat{x}, \hat{y}] = [\hat{y}, \hat{z}] = [\hat{z}, \hat{x}] = 0$$

$$[P_x, P_y] = [\hat{P}_y, \hat{P}_z] = [\hat{P}_z, \hat{P}_x] = 0$$

$$[\hat{x}, \hat{P}_x] = i\hbar = [\hat{y}, \hat{P}_y] = [\hat{z}, \hat{P}_z]$$

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$

$$[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$$

$$[\hat{L}_z, \hat{L}_x] = i\hbar L_y$$

$$[\hat{x}, \hat{L}_x] = 0$$

$$[x, L_y] = i\hbar \hat{z}$$

$$[x, L_z] = -i\hbar y$$

$(L^2, \vec{L})$

$$[L_x, L_y] = [yP_z - zP_y, zP_x - xP_z]$$

$$= [(yP_z), zP_x] + [(zP_y), xP_z]$$

$$= [yP_z, z]P_x + x[zP_y, P_z] = y\underbrace{[P_z, z]}_{-i\hbar}P_x + x\underbrace{[z, P_z]}_{i\hbar}P_y$$

$$= i\hbar[xP_y - yP_x] = i\hbar P_z$$

L^2 which might commute

$$\vec{L}^2 = \hat{L}_x\hat{L}_x + \hat{L}_y\hat{L}_y + \hat{L}_z\hat{L}_z$$

$$[\hat{L}_x, \vec{L}^2] = [L_x, L_xL_x + L_yL_y + L_zL_z]$$

$$= \underbrace{[L_x, L_y]}_{i\hbar L_z}L_y + L_y\underbrace{[L_x, L_y]}_{i\hbar L_z} + \underbrace{[L_x, L_z]}_{-i\hbar L_y}L_z + L_z\underbrace{[L_x, L_z]}_{-i\hbar L_y}$$

$$= 0 \Rightarrow [\hat{L}_y, \vec{L}^2] = [\hat{L}_z, \vec{L}^2] = 0 \Rightarrow [L^2, L] = 0$$

$$[\hat{J}_x, \hat{J}_y] = i\hbar J_z$$

$$[\hat{J}_y, \hat{J}_z] = i\hbar \hat{J}_x$$

$$[\hat{J}_z, \hat{J}_x] = i\hbar \hat{J}_y$$

Donot commute.

$\Rightarrow$ since J^2 is invariant under rotation

$$[\hat{J}^2, J_x] = [J^2, \hat{J}_y] = [\hat{J}^2, \hat{J}_z] = 0$$

J^2, J_x, J_y, J_z canhave same eigen angular moment

J_z not special

$$\hat{J}^2|jm\rangle = j(j+1)\hbar^2|jm\rangle$$

$$\hat{J}_z|j,m\rangle = m\hbar|jm\rangle$$

eigenvalue eqns

where value of j =

$j = 0, 1/2, 1, 3/2, \ldots$

$m = -j$ to $+j$

$= i\hbar\hat{z}$

$= -i\hbar\hat{y}$

$[\hat{P}_x, \hat{L}_x] = 0$

$[\hat{P}_x, L_y] = i\hbar p_z$

$[P_x, L_z] = -i\hbar p_y$

(L^2, L_x) ... invariant under rotation

(P^2, L_z) ... 0

(r^2, L_z) 0

$[\hat{x}, \hat{L}^2] = ? \; [\hat{x}, L_x^2] + [\hat{x}, L_y^2] + [\hat{x}, L_z^2]$

$i\hbar(L_y\hat{z} + \hat{z}L_y - L_z ...)$

$[\hat{P}_x, L^2] = ?$

$[\hat{P}_x, L_x^2] + [\hat{P}_x, \hat{L}_y^2] + [\hat{P}_x, \hat{L}_z^2]$

$i\hbar(\hat{L}_y\hat{P}_z + \hat{L}_y\hat{P}_z - L_zP_y - P_yL_y)$

General theory of angular momentum

$\bar{J}, \bar{J}^2$, angular momentum (Simple angular momentum)

J_x, J_y, J_z, J_+, J_-, rising & lower: components.

($L = \sqrt{l(l+1)}\hbar$, $L_z = m_l\hbar$)

$[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z$
$[\hat{J}_y, \hat{J}_z] = i\hbar\hat{J}_x$ } Do not commute.
$[\hat{J}_z, \hat{J}_x] = i\hbar\hat{J}_y$

⟹ Since J^2 is invariant under rotation

$[\hat{J}^2, J_x] = [J^2, \hat{J}_y] = [\hat{J}^2, \hat{J}_z] = 0$ separately

J^2, J_x, J_y, J_z can have same eigen angular moment.
J_z not special

$\hat{J}^2|j,m\rangle = j(j+1)\hbar^2|j,m\rangle$ ✓

$\hat{J}_z|j,m\rangle = m\hbar|j,m\rangle$ ✓

eigenvalue eqns ✓

Where value of $j =$

$j = 0, 1/2, 1, 3/2 \ldots$

$m = -j$ to $+j$

or $\sqrt{j(j+1) - m(m\pm 1)}\hbar$

$$J_+|j,m\rangle = \sqrt{(j-m)(j+m+1)}\,\hbar\,|j,m+1\rangle$$

$$J_-|j,m\rangle = \sqrt{(j+m)(j-m+1)}\,\hbar\,|j,m-1\rangle$$

where $J_\pm = \hat{J}_x \pm i\hat{J}_y$

$$J_x = \frac{1}{2}(J_+ + J_-) \; ; \; J_y = \frac{1}{2i}(J_+ - J_-)$$

$J_+ = J_x + iJ_y$

$J_- = J_x - iJ_y$

$(J_+ + J_-) = 2J_x$

$(J_+ - J_-) = 2iJ_y$

Matrix form of Different Angular momentum Operator

orthogonal

$$\sum_{m=-j}^{+j} |j,m\rangle\langle j,m| = I$$

$$\langle j',m'|J^2|j,m\rangle = \hbar^2\, j(j+1)\,\delta_{j',j}\,\delta_{m',m}$$

$$\langle j',m'|J_z|j,m\rangle = m\hbar\,\delta_{j',j}\,\delta_{m',m}$$

$$\langle j',m'|J_\pm|j,m\rangle = \hbar\sqrt{(j\mp m)(j\pm m+1)}\,\delta_{j',j}\,\delta_{m',m\pm 1}$$

$$\langle j',m'|J_-|j,m\rangle = \hbar\sqrt{(j+m)(j-m+1)}\,\delta_{j',j}\,\delta_{m',m-1}$$

$$\langle j',m'|J_x|j,m\rangle = \frac{1}{2}(J_+ + J_-)$$

$$\langle j',m'|J_y|j,m\rangle = \frac{1}{2i}(J_+ - J_-) \text{ or } \frac{i}{2}(J_- - J_+)$$

Problem

let $j=1$ find out the matrixes for $J^2, J_z, J_\pm, J_x, J_y$

Ans) for $j=1$ $m = 1, 0, -1$

Possible joint eigen state are for J^2

$|jm\rangle \Rightarrow |1,1\rangle, |1,0\rangle, |1,-1\rangle$

3 eigen states $\Rightarrow$ 3×3 matrix

matrix element for J^2

$$J^2 = \begin{bmatrix} \langle 1\,1|J^2|11\rangle & \langle 1\,1|J^2|10\rangle & \langle 1\,1|J^2|1\,-1\rangle \\ \langle 1\,0|J^2|11\rangle & \langle 1\,0|J^2|10\rangle & \langle 1\,0|J^2|1\,-1\rangle \\ \langle 1\,-1|J^2|11\rangle & \langle 1\,-1|J^2|10\rangle & \langle 1\,-1|J^2|1\,-1\rangle \end{bmatrix}$$

$\langle j'm'|J^2|jm\rangle = j(j+1)\hbar^2 \delta_{j'j}\delta_{m'm}$ } General

Diagonal element finite

$$J^2 = \hbar^2 \begin{bmatrix} 1(1+1)=2 & 0 & 0 \\ 0 & 2=1(1+1) & 0 \\ 0 & 0 & 1(1+1)=2 \end{bmatrix}$$

$$J^2 = 2\hbar^2 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$J_z = \langle j'm' | J_z | jm \rangle = m\hbar\, \delta_{j'j}\, \delta_{m'm}$$

$$J_z = \hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

(m)

eigen eqn

$$J_z | jm \rangle = m\hbar | jm \rangle$$

for matrix elemt

$$\langle j'm' | J_z | jm \rangle = m\hbar \langle j'm' | jm \rangle$$

$$\langle j'm' | J_- | jm \rangle = \hbar \sqrt{(j+m)(j-m+1)}\, \delta_{j'j}\, \delta_{m'm-1}$$

matrix

$$J_- = \hbar \begin{bmatrix} 0 & 0 & 0 \\ \sqrt{(1+1)(1-1+1)} = \sqrt{2} & 0 & 0 \\ 0 & \sqrt{(1+0)(1-0+1)} = \sqrt{2} & 0 \end{bmatrix}$$

$$= \sqrt{2} \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

or $\sqrt{j(j+1) - m(m-1)}\ \hbar$

$= \sqrt{1(2) - 1(0)}$

$= \sqrt{2}$

$\langle j m' | J_+ | j m \rangle = \hbar \sqrt{(j-m)(j+m+1)}$

...ning joint Eigen state for $\hat{J}^2$ & $\hat{J}_z$

$\hat{J}_z |j,m\rangle = m\hbar |j,m\rangle$

$$\hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = m\hbar \begin{pmatrix} a \\ b \\ c \end{pmatrix} \Rightarrow \begin{matrix} \hbar a = m\hbar a \\ 0 = m\hbar b \\ -\hbar c = m\hbar c \end{matrix}$$

Normalized solution to these eqn for $m = 1, 0, -1$

$$|1,1\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \quad |1,0\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \quad |1,-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

they are orthonormal $\Rightarrow \langle 1, m' | 1, m \rangle = \delta_{m'm} \Rightarrow (m, m') = (-1, 0, 1)$

completness $\sum_{m=-1}^{1} |1,m\rangle\langle 1,m| = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

$$\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$= \sqrt{2}$

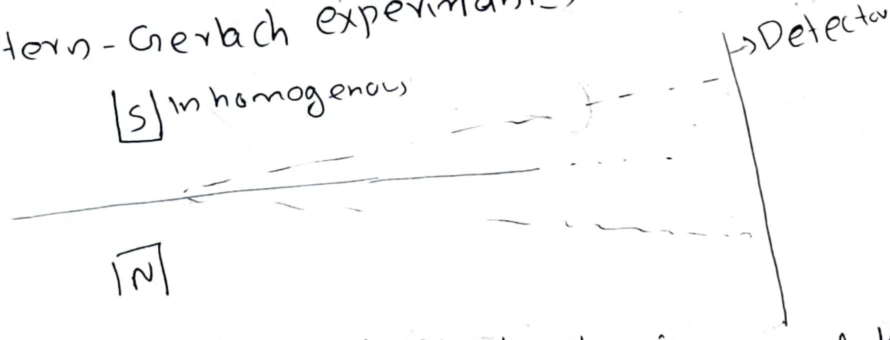
$\sqrt{j(j+1) - m(m-1)}\ \hbar$

$= 1(2) - 1(0)$

$\sqrt{2}$

General theory of spin

Stern-Gerlach experimant $\Rightarrow$



If a neutral beam of silver atom is passed through homogenous magnetic field then Beam split into ... parts. Due to the Interaction of magneti...

$J_+ \Rightarrow \langle j'm'|J_+|jm\rangle = \hbar\sqrt{(j-m)(j+m+1)}\,\delta_{j'j}\,\delta_{m',m+1}$

$$J_+ = \hbar\begin{bmatrix} 0 & \sqrt{(1-0)(1+0+1)}=\sqrt{2} & 0 \\ 0 & 0 & \sqrt{(1-1)(1-1+0)}=\sqrt{2} \\ 0 & 0 & 0 \end{bmatrix}$$

$$J_+ = \sqrt{2}\hbar\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

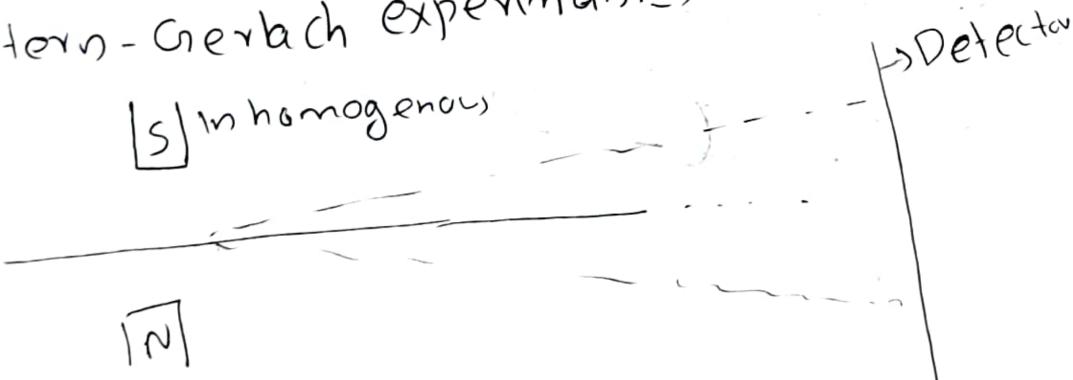
J_x & J_y

$J_x = \frac{1}{2}[J_+ + J_-] \Rightarrow \quad J_x = \frac{\hbar}{\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$

$J_y = \frac{1}{2i}[J_+ - J_-] \Rightarrow \quad J_y = \frac{\hbar}{\sqrt{2}}\begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix}$

General theory of spin

Stern-Gerlach experimant ⇒



If a neutral beam of silvel atom is passed thrugh In homogenous magnetic field then Beam split into 2 parts Due to the Interaction of magneti momentum

and magnetic field.

Beam will split into $(2l+1)$ parts.

$L_x = m_l \hbar$, $m_L = -l$ --- to ... $+l$.

when Ag atom is in groundstate $l=0$ then beam split into 1

when we consider electron spin $(1/2)$, the angular momentum $S = (l \pm 1/2) \Rightarrow 1/2 ; 1/2$

Spacitial orientation of the Angular momentum is Quantized.

General Theory of spin (~~excluding~~ $\hbar$ for simplicity)

$J \xrightarrow{\text{likes}} S$ $\quad S_x, S_y, S_z, S^2$

$[\hat{S}_x, \hat{S}_y] = i\hbar S_z$; $[\hat{S}_x, \hat{S}_y] = i\hbar S_x$; $[\hat{S}_z, \hat{S}_x] = i\hbar \hat{S}_y$

$[S^2, S_z] = 0$, $\Rightarrow$ common eigen state.

Eigen value eqn

$\hat{S}^2 |s, m_s\rangle = \hbar^2 s(s+1)|s, m_s\rangle$; $\hat{S}_z |s, m_s\rangle = m_s\hbar |s, m_s\rangle$

$(s+1) \dots (s-1)_z$

or $\hbar\sqrt{s(s+1) - m_s(m_s \pm 1)}$, $m_s = -s$ to $+s$

$\hat{S}_+ |s, m_s\rangle = \hbar\sqrt{(s-m_s)(s+m_s+1)}\, |s, m_s+1\rangle$ because raising op

$\hat{S}_- |s, m_s\rangle = \hbar\sqrt{(s+m_s)(s-s_m+1)}\, |s, m_s-1\rangle$

$\left(S_\pm = S_x \pm i S_y\right)$

$\hat{S}_x = \frac{1}{2}(\hat{S}_+ + \hat{S}_-)$;

$\hat{S}_y = \frac{1}{2i}(\hat{S}_+ - \hat{S}_-) = \frac{i}{2}(\hat{S}_- - \hat{S}_+)$

let spin $s = 1/2$, find out $\hat{S}^2$, $\hat{S}_x$, $\hat{S}_y$, $\hat{S}_z$, $\hat{S}_+$, $\hat{S}_-$

$s = \frac{1}{2}$, $m_s = \frac{1}{2}\ -\frac{1}{2}$

$|s, m_s\rangle = |\frac{1}{2}, \frac{1}{2}\rangle ; |\frac{1}{2}, -\frac{1}{2}\rangle$ 2x2 matrix

General

$$S^2 = \begin{bmatrix} \langle \frac{1}{2}\ \frac{1}{2}| S^2 | \frac{1}{2}\ \frac{1}{2}\rangle & \langle \frac{1}{2}\ \frac{1}{2}| S^2 | \frac{1}{2}\ -\frac{1}{2}\rangle \\ \langle \frac{1}{2}\ -\frac{1}{2}| S^2 | \frac{1}{2}\ \frac{1}{2}\rangle & \langle \frac{1}{2}\ -\frac{1}{2}| S^2 | \frac{1}{2}\ -\frac{1}{2}\rangle \end{bmatrix}$$

$$\langle s' m_s' | S^2 | s\, m_s\rangle = s(s+1)\hbar^2\, \delta_{s's}\, \delta_{m_s' m_s}$$

$$S^2 = \hbar^2 \begin{bmatrix} 3/4 & 0 \\ 0 & \frac{3}{4} \end{bmatrix} = \frac{3\hbar}{4} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\langle s' m_s' | S_z | s\, m_s\rangle = m_s \hbar\, \delta_{s's}\, \delta_{m_s' m}$$

$$S_z = \hbar \begin{bmatrix} 1/2 & 0 \\ 0 & -1/2 \end{bmatrix} = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \frac{\hbar}{2}\sigma_z$$

$$\langle s' m_s' | S_\pm | s m_s \rangle = \hbar \sqrt{(s \mp m_s)(s \pm m_s + 1)} \; \delta_{ss'} \delta_{m_s' m_s \pm 1}$$

$$s(s+1) - m_s(m_s \pm 1)$$

$$\tfrac{1}{2}(\tfrac{1}{2}+1) + \tfrac{1}{2}(\tfrac{1}{2}+1)$$

$$\tfrac{3}{4} + \tfrac{1}{4} = [illegible]$$

$$S_+ = \hbar \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

$$S_- = \hbar \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \qquad \sqrt{(\tfrac{1}{2}+\tfrac{1}{2})(\tfrac{1}{2}-\tfrac{1}{2}+1)}\,\hbar$$

σ_m … S_z … $\frac{\hbar}{2}$ … m_s

$$S_x = \frac{1}{2}(S_+ + S_-) = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Rightarrow \frac{\hbar}{2}\sigma_x$$

$$S_y = \frac{i}{2}(S_- - S_+) = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \frac{\hbar}{2}\sigma_y$$

Pauli matrix $(\sigma_x, \sigma_y, \sigma_z)$

$$\boxed{\vec{S} = \frac{\hbar}{2}\vec{\sigma}}$$

$$\Rightarrow \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\langle s' s m_s' | S_\pm | s m_s \rangle = \hbar \sqrt{(s \mp m)(s \pm m + 1)}\, \delta_{s's}\, \delta_{m_s' m_{s\pm}}$$

$$s(s+1) - m_s(m_s+1)$$

$$\frac{1}{2}\left(\frac{1}{2}+1\right) + \frac{1}{2}\left(-\frac{1}{2}+1\right)$$

$$\frac{3}{4} + \frac{1}{4} = \frac{4}{4}$$

$$S_+ = \hbar \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

$$S_- = \hbar \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

$$\sqrt{\left(\frac{1}{2}+\frac{1}{2}\right)\left(\frac{1}{2}-\frac{1}{2}+1\right)}\,\hbar$$

Joint

$S_z |$

$\frac{\hbar}{2}$

$|s, m_s\rangle$

Yes they

$$S_x = \frac{1}{2}(S_+ + S_-) = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Rightarrow \frac{\hbar}{2}\sigma_x$$

$$S_y = \frac{i}{2}(S_- - S_+) = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \frac{\hbar}{2}\sigma_y$$

Pauli matrix $(\sigma_x, \sigma_y, \sigma_z)$

$$\boxed{\vec{S} = \frac{\hbar}{2}\vec{\sigma}}$$

$$\Rightarrow \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Properties

Joint Eigen vector of $\hat{S}^2$ & $\hat{S}_z$

$S_z|s, m_s\rangle = m_s\hbar|s, m_s\rangle$

$\frac{\hbar}{2}\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}\begin{bmatrix}a\\b\end{bmatrix} = m_s\hbar\begin{bmatrix}a\\b\end{bmatrix} \Rightarrow \frac{\hbar}{2}a = m_s\hbar a$

$-\frac{\hbar}{2}b = m_s\hbar b$

$|s, m_s\rangle \Rightarrow |\frac{1}{2}, \frac{1}{2}\rangle = \begin{bmatrix}1\\0\end{bmatrix}$; $|\frac{1}{2}, -\frac{1}{2}\rangle = \begin{bmatrix}0\\1\end{bmatrix}$

Yes they are complete & orthonormal.

with a tensor of x, y, z ... zero

$\sigma_j\sigma_k = \delta_{jk} + i\sum_l \varepsilon_{jkl}$

Addition of Angular momenta ($J_1 + J_2$)

2 System J_1 J_2

$[\hat{J}_1^2, \hat{J}_{1z}] = 0 \Rightarrow |j_1 m_1\rangle$ $|j_2 m_2\rangle \leftarrow [J_2^2, J_{2z}] = 0$

simultaneous eigen|> of $\hat{J}_1^2$ and $\hat{J}_{1z}$, similarly J_2^2 & J_{2z}

$J_1^2|j_1 m_1\rangle = j_1(j_1+1)\hbar^2|j_1 m_1\rangle$ → will have $(2j+1)$ dimension (states)

eg: $|j_1, -j\rangle, |j_1, -j+1\rangle, \ldots |j_1, j\rangle$

$J_{1z}|j_1 m_1\rangle = m_1\hbar|j_1 m_1\rangle$

$J_2^2|j_2 m_2\rangle = j_2(j_2+1)\hbar^2|j_2 m_2\rangle$

$J_{2z}|j_2 m_2\rangle = m_2\hbar|j_2 m_2\rangle$

$m_1 = j_1 \ldots -j_1$

$m_2 = j_2 \ldots -j_2$

we have $[\hat{J}_1, \hat{J}_2] = 0$, Because they belong to different states

$[J_1^2, J_2^2] = 0$

Properties

$\sigma_j^2 = I$, $(j = x, y, z)$

$\sigma_j \sigma_x + \sigma_x \sigma_j = 0$ anticommute

$\{\sigma_j, \sigma_k\} = 2\hat{I}\,\delta_{jk}$

$[\sigma_j, \sigma_k] = 2i\,\epsilon_{jkl}\,\sigma_l$, ϵ_{jkl} = levi-Civita tensor

$$\epsilon_{ijk} = \begin{cases} 1 = \text{even permutation of } (x,y,z) \\ -1 = \text{odd permutation} \\ 0 = 2 \text{ indices are zero} \end{cases}$$

$\sigma_j \sigma_k = \delta_{jk} + i \sum_l \epsilon_{jkl}$

Addition of Angular momenta $(J_1 + J_2)$

2 System J_1 J_2

$[J_1^2, J_{1z}] = 0 \Rightarrow |j_1 m_1\rangle$ simultaneous eigen $|\rangle$ of $\hat{J}_1^2$ and $\hat{J}_{1z}$

$|j_2 m_2\rangle \Leftarrow [J_2^2, J_{2z}] = 0$ similarly J_2^2 & J_{2z}

$J_1^2 |j_1 m_1\rangle = j_1(j_1+1)\hbar^2 |j_1 m_1\rangle$

$J_{1z} |j_1 m_1\rangle = m_1\hbar\, |j_1 m_1\rangle$

will have $(2j+1)$ dimension (states)

eg: $|j_1, -j\rangle, |j_1, -j+1\rangle, \ldots |j_1, j\rangle$

$J_2^2 |j_2 m_2\rangle = j_2(j_2+1)\hbar^2 |j_2 m_2\rangle$

$J_{2z} |j_2 m_2\rangle = m_2\hbar\, |j_2 m_2\rangle$

$m_1 = j_1 \ldots -j_1$

$m_2 = j_2 \ldots -j_2$

we have $[\hat{J}_1, \hat{J}_2] = 0$, Because they belong to different states

$[J_1^2, J_2^2] = 0$

$J_1^2, J_{1z}, J_2^2, J_{2z}$ } they will commute so they have common eige (or joint)

* Common eigenstate $|j_1 m_1\rangle |j_2, m_2\rangle$ (known)

$|j_1 j_2; m_1, m_2\rangle$ ═══

So we can rewrite the privious eqns in these eigen states ⇒

Totel Angular momentum

$J = J_1 + J_2$ | $[\hat{J}_x, J_y] = i\hbar J_z$, $[\ ,\ ] =$ Cyclic Permutation

we have $[J^2, J_z] = 0$, $= [J_1^2, J_z] = [J_z^2, J_z]$, $[J^2, J_1^2] = [J^2, J_2^2] = 0$

$|j\, m\rangle$ $|j_1 j_2\rangle$ but $[\hat{J}^2, J_{1z}] \neq 0$

$[\hat{J}^2, \hat{J}_{2z}] \neq 0$

Common Eigenstates $(\hat{J}_1^2, \hat{J}_2^2, J^2, J_z)$ They will commute seperaty ^Common eigen state

$|j_1 j_2; j, m\rangle$ (unknown)

Check above page bottom

let's represent unknon eisenstate $(|j_1 j_2 j\, m\rangle)$ in term of known state $|j_1 j_2; m_1, m_2\rangle$

via linear combination

unknown, linear combination, known state

$$|j, m\rangle = \sum_{m_1, m_2} C_{jm, m_1, m_2} |m_1, m_2\rangle$$

rep ① Clebsh-Gorden CG coe

Wigner coe

CG coe are Unitary. $U^\dagger = U^{-1}$

$J_1^2, J_{1z}, J_2^2, J_{2z}$] they will commute so they have common eigen (or joint)

Denote common eigenstate $|j_1 m_1\rangle|j_2, m_2\rangle$ (known)

$$\hat{J}_1^2 |j_1 j_2; m_1, m_2\rangle = j_1(j_1+1)\hbar^2 |j_1, j_2; m_1 m_2\rangle$$

$$\hat{J}_{1z} |j_1, j_2; m_1, m_2\rangle = m_1\hbar |j_1, j_2; m_1 m_2\rangle$$

$$\hat{J}_2^2 |j_1, j_2; m_1, m_2\rangle = j_2(j_2+1)\hbar^2 |j_1, j_2; m_1, m_2\rangle$$

$$J_{2z} |j_1, j_2; m_1, m_2\rangle = m_2\hbar |j_1, j_2; m_1 m_2\rangle$$

---

yes there are orthonormal & complete.

orthogonality $\langle \mid \rangle = \delta_{j_1' j_1} \delta_{j_2' j_2} \delta_{m_1' m_1} \delta_{m_2' m_2}$

completeness $\sum_{m_1 m_2} |\ ;\ \rangle \langle\ | = 1 = \left(\sum_{m_1} |j_1 m_1\rangle\langle\ |\right)\left(\sum_{m_2} |j_2 m_2\rangle\langle\ |\right)$

Total Dimension $\Rightarrow N = 2(j_1+1) \times (2j_2+1)$

$$J_{1\pm} |j_1, j_2; m_1, m_2\rangle = \hbar\sqrt{(j_1 \mp m_1)(j_1 \pm m_1 + 1)}\ |j_1, j_2; m_1 \pm 1, m_2\rangle$$

or $\sqrt{j_1(j_1+1) - m_1(m_1 \pm 1)}$

$$J_{2\pm} |j_1 \quad \rangle = \hbar\sqrt{(j_2 \mp m_2)(\quad)}\ |j_1, j_2; m_1, m_2 \pm 1\rangle$$

$J_x = \frac{1}{2}(J_+ + J_-)$ $\quad J_y = \frac{1}{2i}(J_+ - J_-)$

---

in term of known state $|j_1, j_2; m_1, m_2\rangle$

linear combination

unknown $\quad$ known state $\quad$ rep

$$|j, m\rangle = \sum_{m_1 m_2} C_{j m, m_1, m_2} |m_1, m_2\rangle$$

① Clebsh-Gordon CG coe

Wigner coe

CG coe are Unitary. $U^\dagger = U^{-1}$

$^2_2, J_{2z}$] they will commute so they have common eigen (or joint)

eigenstate. $|j_1 m_1\rangle |j_2, m_2\rangle$ (known)

$_1, m_2\rangle$ ==

rewrite the privious eqns in these eigen

---

gular momentum — cyclic [...]

$J_1 + J_2$ | $[\hat{J}_x, J_y] = i\hbar J_z$, $[\ ,\ ] = i[\ ,\ ]$

$_z] = 0$; $= [J_1^2, J_z] = [J_2^2, J_z]$

$[J^2, J_1^2] = [J^2, J_2^2] = 0$

but $[\hat{J}^2, J_{1z}] \neq 0$

$[\hat{J}^2, \hat{J}_{2z}] \neq 0$

$m\rangle$ $|j_1 j_2\rangle$

$, J_z)$ They will commute seperately

common eigen state

$|j_1 j_2; j, m\rangle$ (unknown)

represent unknon eigenstate ($|j_1 j_2 j m\rangle$) in term of known state $|j_1 j_2 m_1, m_2\rangle$

linear combination

unknown — known state

$$|j, m\rangle = \sum_{m_1 m_2} C_{j m, m_1, m_2} |m_1, m_2\rangle$$

① Clebsh-Gordon CG coe

wigner coe

CG coe are Unitary. $U^\dagger = U^{-1}$

$\hat{J}_1^2 |j_1, j_2; j, m\rangle = j_1(j_2+1)\hbar^2 |j_1, j_2; j, m\rangle$

$\hat{J}_2^2 |\ \ \rangle = j_2(j_2+1)\hbar^2 |\ \ \rangle$

$\hat{J}^2 |\ \ \rangle = j(j+1)\hbar^2 |\ \ \rangle$

$\hat{J}_z |\ \ \rangle = m\hbar |\ \ \rangle$

yes complete $\sum_j \sum_{m=-j}^{j} |\ \ \rangle\langle\ \ | = 1$

$\langle\ \ |\ \ \rangle = \delta_{j'j}\delta_{m'm}$

orthogonal

$N = (2j_1+1) * 2(j_2+1)$

... J_2^2, J_{2z}] they will ... they have ... (or ...

... en eigenstate $|j_1 j_2; m_1 m_2\rangle$ = $|j, m\rangle$

So we can rewrite the pri...

states ⇒ Total Angular

$J = J_1 + J_2$

we have $[J^2, J_2^2]$ ...

common eigenstate

New aim : calculate coe

$\langle m_1 m_2 |$ $|jm\rangle = \mathbb{I}\,|jm\rangle$

We have to ... unknown state ... state

① $\Rightarrow \langle m_1 m_2 | j m\rangle = C_{j,m,m_1,m_2}$

$$\Rightarrow |j,m\rangle = \sum_{m_1 m_2} |m_1 m_2\rangle\langle m_1 m_2 | j m\rangle$$

coe to know, unknown to k ... — ②

(unique)

or Full thing

$$|j_1 j_2 ; j m\rangle = \sum_{m_1 m_2} |j_1 j_2 ; m_1 m_2\rangle\langle j_1 j_2 ; m_1 m_2 | j_1 j_2 ; j m\rangle$$

Before that

Selection Rule:

From eqn ②

$$J_z |j,m\rangle = \sum_{m_1 m_2} (J_{1z} + J_{2z}) |m_1 m_2\rangle\langle m_1 m_2 | j m\rangle$$

$$m\hbar |j,m\rangle = \sum_{m_1 m_2} (m_1 + m_2)\hbar\, |m_1 m_2\rangle\langle m_1 m_2 | j m\rangle \quad — ③$$

($|jm\rangle$)

Put ② in ③ and re-arrange

$\Rightarrow$

$$\sum_{m_1 m_2} (m_1 + m_2 - m) |m_1 m_2\rangle\langle m_1 m_2 | j m\rangle = 0$$

coe cannot be zero.

$\Rightarrow m_1 + m_2 - m = 0$

$$\boxed{m = m_1 + m_2}$$

$|j_1 - j_2| \le j \le |j_1 + j_2|$

Selection rule

$j_1 \Rightarrow m_1 = (-j_1 \ldots j_1)$

$m_2 = (-j_2 \ldots j_2)$

another condition

~~cor~~ orthonormal condition

$$\sum \left| \langle j_1 j_2 ; m_1 m_2 | j m \rangle \right|^2 = 1$$

for simplicity $\Rightarrow \left| \langle m_1 m_2 | j m \rangle \right|^2 = 1$

also ~~CG coe for unitary for~~

CG coe form a unitary matrix

$U^{+} = U^{-1}$

—

Problem: Find the CG Coe ~~Asos~~ Associated with the coupling of spins of the electron & proton of an Hydrogen Atom in its ground states b) Find transformation matrix & check unitary.

$j_1 = 1/2 \; ; \; j_2 = 1/2$

value of $j = j_1 \pm j_2 \Rightarrow (0 \text{ or } 1)$

...ble

states in terms of known stat.

$\sum |m_1 m_2\rangle \langle m_1 m_2 | j m \rangle$

$\sum_{m_1 m_2} \underbrace{\langle j_1 j_2 ; m_1 m_2 | j m \rangle}_{\text{CG coes}} \; \underbrace{| j_1 j_2 ; m_1 m_2 \rangle}_{\text{known}}$

$m = 0 \quad \Rightarrow |j, m\rangle = |0, 0\rangle$

$m = -1, 0, +1 \quad |j m\rangle = |1, 1\rangle, |1, 0\rangle, |1, -1\rangle$

...ies ~~de~~ need to be describ...

unknown

...ms of ... States $(m_1 m_2)$

another condition:

~~cos~~ orthonormal condition

$$\sum \left| \langle j_1 j_2 ; m_1 m_2 | j m \rangle \right|^2 = 1$$

for simplicity $\Rightarrow \left| \langle m_1 m_2 | j m \rangle \right|^2 = 1$

also ~~CG coe for unitary for~~

CG coe form a unitary matrix

$$U^{+} = U^{-1}$$

—

Problem: Find the CG coe ~~Asos~~ Associated with the coupling of spins of the electron a) and proton of an Hydrogen Atom in its ground states b) Find transformation matrix & check unitary.



$$j_1 = \frac{1}{2} \; ; \; j_2 = \frac{1}{2}$$

Possible value of $j = j_1 \pm j_2 \Rightarrow (0 \text{ or } 1)$

unknown state, in terms of known state.

~~$|jm\rangle = \sum |m_1 m_2\rangle \langle m_1 m_2 | jm\rangle$~~

$$\underbrace{|jm\rangle}_{\text{unknown}} = \sum_{m_1 m_2} \underbrace{\langle j_1 j_2 ; m_1 m_2 | jm \rangle}_{\text{CG coes}} \underbrace{|j_1 j_2 ; m_1 m_2\rangle}_{\text{known}}$$

$j = 0 \; ; \; m = 0 \quad \Rightarrow |jm\rangle = |0,0\rangle$

$j = 1 \; ; \; m = -1, 0, +1 \quad = |jm\rangle = |1,1\rangle, |1,0\rangle, |1,-1\rangle$

Thee ~~4~~ unknown states ~~are~~ need to be described interms of ~~4~~ known states $(m_1 m_2)$

$|0,0\rangle = \langle \tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{-1}{2}|0,0\rangle\, |\tfrac{1}{2}\tfrac{1}{2};\ \tfrac{1}{2}\tfrac{-1}{2}\rangle +$

(under the terms: m; j_1, j_2; m_1, m_2; j, m)

$j_2 = j_1 = \tfrac{1}{2} \Rightarrow m_1 = m_2 \left(-\tfrac{1}{2}, +\tfrac{1}{2}\right)$

selection rule $\Rightarrow m_1 + m_2 = m$

$\Rightarrow \left(\tfrac{1}{2} + \tfrac{1}{2}\right) \neq 0 = \left(\tfrac{1}{2} - \tfrac{1}{2}\right)$

$\langle \tfrac{1}{2},\tfrac{1}{2};\ \tfrac{-1}{2},\tfrac{1}{2}|00\rangle\, |\tfrac{1}{2}\tfrac{1}{2};\ \tfrac{-1}{2},\tfrac{1}{2}\rangle$ — (2)

— (3)

$|1,1\rangle = \langle \tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2}\tfrac{1}{2}|11\rangle\, |\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2}\tfrac{1}{2}\rangle$

$|1,0\rangle = \langle \tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{-1}{2}|1,0\rangle\, |\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2}\tfrac{-1}{2}\rangle +$

$\langle \tfrac{1}{2},\tfrac{1}{2};\ \tfrac{-1}{2}\tfrac{1}{2}|1,0\rangle\, |\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{-1}{2}\tfrac{1}{2}\rangle$ — (4)

$|1,-1\rangle = \langle \tfrac{1}{2},\tfrac{1}{2};\ -\tfrac{1}{2},\tfrac{-1}{2}|1,-1\rangle\, |\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{-1}{2},\tfrac{-1}{2}\rangle$ — (5)

(CG coe to be determined)

$\langle 11|11\rangle = 1$

from eqn (3) $|1,1\rangle$ ($j\ m$) ; $|\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2}\rangle$ are normalized

orthonormal condition $|\langle \tfrac{1}{2}\tfrac{1}{2};\ \tfrac{1}{2}\tfrac{1}{2}|1,1\rangle|^2 = 1$

$\Rightarrow \langle \tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2}|11\rangle = 1$

(3) $\Rightarrow |1,1\rangle = a\,|\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2}\rangle$ — (6)

$j = 1$
$m = 1$
$j_1 = \tfrac{1}{2} = m_1$
$j_2 = \tfrac{1}{2} = m_2$
$m = m_1 + m_2$
$= j_1 + j_2$

apply J_- on (6)

$J_-|11\rangle = (J_{1-} + J_{2-})|\tfrac{1}{2}\tfrac{1}{2};\ \tfrac{1}{2}\tfrac{1}{2}\rangle$

($j\ m$; $j_1\ j_2$; $m_1\ m_2$)

$j(j+1) - m(m-1)$

$J_-|jm\rangle = \sqrt{j\pm m(j-m+1)}\,|j,m-1\rangle$

Previous page

$\hbar\sqrt{2}|10\rangle = \hbar 1\,|\tfrac{1}{2}\tfrac{1}{2};\ \tfrac{-1}{2}\tfrac{1}{2}\rangle + 1\,|\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2}\tfrac{-1}{2}\rangle$

$\Rightarrow |1,0\rangle = \frac{1}{\sqrt{2}} \left| \frac{1}{2}\frac{1}{2} ; -\frac{1}{2}\frac{1}{2} \right\rangle + \frac{1}{\sqrt{2}} \left| \frac{1}{2}\frac{1}{2} ; \frac{1}{2} -\frac{1}{2} \right\rangle$

(j, m; $j_1\ j_2$; $m_1\ m_2$)

comparing ⑦ & ② $\Rightarrow \left\langle \frac{1}{2}\frac{1}{2} ; -\frac{1}{2}\frac{1}{2} \right| = \frac{1}{\sqrt{2}}$

$\left\langle \frac{1}{2}\frac{1}{2} ; \frac{1}{2} -\frac{1}{2} \right| = \frac{1}{\sqrt{2}}$

~~ap~~ apping J_- on ⑦ $\Rightarrow$

$\sqrt{2}|1\ -1\rangle = \frac{1}{\sqrt{2}} \left[0 \left| \frac{1}{2}\frac{1}{2} ; -\frac{3}{2}\frac{1}{2} \right\rangle + 1 \left| \frac{1}{2}\frac{1}{2} ; -\frac{1}{2} -\frac{1}{2} \right\rangle \right]$

$\sqrt{\frac{1}{2}\left(\frac{3}{2}\right) + \frac{1}{2}\left(-\frac{3}{2}\right)} = 0$

$J_-|jm\rangle = \sqrt{(j+m)(j-m+1)}|j$

$= 1 \times (1-0+1)$

$1 \times 2 = \sqrt{2}|1\ -1\rangle$

$\sqrt{\frac{1}{2} \cdot \frac{1}{2}\left(\frac{1}{2} - \frac{1}{2} + 1\right)}$ ~~=~~ 0

$+ \frac{1}{\sqrt{2}} \left[1 \left| \frac{1}{2}\frac{1}{2} ; -\frac{1}{2} -\frac{1}{2} \right\rangle + 0 \left| \frac{1}{2}\frac{1}{2} ; \frac{1}{2} -\frac{3}{2} \right\rangle \right]$

$= \frac{1}{\sqrt{2}} \left[2 \left| \frac{1}{2}\frac{1}{2} ; -\frac{1}{2} -\frac{1}{2} \right\rangle \right]$

$|1,-1\rangle = 1 \left| \frac{1}{2}\frac{1}{2} ; -\frac{1}{2} -\frac{1}{2} \right\rangle$ — ⑧

⑧ & ⑤ $\Rightarrow$ CG coe $= 1$

No cannot just apply $J_\pm$ to obtain $|0\,0\rangle$

② $\Rightarrow$

$|0,0\rangle = a \left| \frac{1}{2}, \frac{1}{2} ; -\frac{1}{2}, \frac{1}{2} \right\rangle + b \left| \frac{1}{2}, \frac{1}{2} ; \frac{1}{2}, -\frac{1}{2} \right\rangle$ — ⑨

a, b } are CG coe tobe determin

To make ⑨ orthonormal

Apply orthonormal condition

orthogonal — $\langle 00|10\rangle = 0$

Normalized $\langle 00|00\rangle = 1$

$\langle 00|10\rangle = \frac{a}{\sqrt{2}} + \frac{b}{\sqrt{2}} = 0 \Rightarrow a = -b$

$\langle 00|00\rangle = a^2 + b^2 = 1 \Rightarrow 2b^2 = 1 \Rightarrow b = \frac{1}{\sqrt{2}}$

$\Rightarrow a = \frac{-1}{\sqrt{2}}$

(9) $\Rightarrow |0,0\rangle = \frac{-1}{\sqrt{2}} \left|\frac{1}{2},\frac{1}{2}; \frac{-1}{2},\frac{1}{2}\right\rangle + \frac{1}{\sqrt{2}} \left|\frac{1}{2},\frac{1}{2}; \frac{1}{2},\frac{-1}{2}\right\rangle$ — (10)

(6), (7), (8), (10)

$|1,1\rangle \; |1,0\rangle \; |1,-1\rangle \; |0,0\rangle$

$|J,m\rangle = [\quad] \; |m_1 m_2\rangle$

unknow — Known

CG coe. — Transformation ma...

$$\begin{bmatrix} |0\,0\rangle \\ |1\,1\rangle \\ |1\,0\rangle \\ |1,-1\rangle \end{bmatrix} = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \left|\frac{1}{2},\frac{1}{2}; \frac{1}{2},\frac{1}{2}\right\rangle \\ \left|\frac{1}{2}\,\frac{1}{2}; \frac{1}{2}\,\frac{-1}{2}\right\rangle \\ \left|\frac{1}{2}\,\frac{1}{2}; \frac{-1}{2}\,\frac{1}{2}\right\rangle \\ \left|\frac{1}{2}\,\frac{1}{2}; \frac{-1}{2}\,\frac{-1}{2}\right\rangle \end{bmatrix}$$

$$U = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$U^{\dagger} = U^{-1}$

Unitary



eg: Coupling of ~~angular~~ orbital momentum of p electron

s, p, d, f

$l = 0$ 1 2 3

GT of A-momenta

$m = -j$ to j)

$$\hat{J}^2 |j,m\rangle = j(j+1)\hbar^2 |j,m\rangle$$

$$\hat{J}_z |j,m\rangle = m\hbar |j,m\rangle$$

$$J_\pm |j,m\rangle = \sqrt{j(j+1) - m(m\pm1)}\ \hbar |j, m\pm1\rangle$$

$$J_\pm = \hat{J}_x \pm i\hat{J}_y \Rightarrow J_x = \frac{1}{2}(J_+ + J_-) \ ; \ J_y = \frac{1}{2i}(J_+ - J_-)$$

eg: $\langle j' m' | J_\pm | j m\rangle = \hbar\sqrt{j(j+1) - m(m\pm1)}\ \delta_{j'j}\delta_{m'\,m\pm1}$

General theory of Spin

$J \rightsquigarrow S$, $j \rightsquigarrow s$, $m \rightsquigarrow m_s$

$$\hat{S} = \frac{\hbar}{2}\vec{\sigma} \qquad \sigma_j^2 = I \qquad j = x, y, z$$

$$\sigma_j\sigma_k + \sigma_k\sigma_j = 0 \Rightarrow \{\sigma_j, \sigma_k\} = 2I\delta_{ij}$$

$$[\sigma_j, \sigma_k] = 2i\,\varepsilon_{jkl}\sigma_l$$

for $S = 1/2$

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\sigma_j\sigma_k = \delta_{jk} + i\sum_l \varepsilon_{jkl}\sigma_l$$

$\sigma_j^\dagger = \sigma_j$, $Tr(\sigma_j) = 0$ $\det(\sigma_j) = -1$,

$\sigma_x\sigma_y\sigma_z = i\hat{I}$ $\qquad \sigma_x\sigma_y = i\sigma_z$

$e^{i\alpha\sigma_j} = I\cos\alpha + i\sigma_j\sin\alpha$.

Addition of Angular moments

dimention $=(2j+1)$ $\quad J_1^2, J_2^2, J_{1z} J_{2z}$ } commute.

eg:

$$J_{1\pm} | j_1 j_2 ; m_1 m_2 \rangle = \sqrt{j(j+1) - m(m\pm1)}\,\hbar\, | j_1 j_2 ; m_1 \pm m_2 \rangle$$

$$J = J_1 + J_2 \Rightarrow J_- = J_{1-} + J_{2-}, \ldots$$

J_1^2, J_2^2, J^2, J_z jointly commute.

but $[J^2, J_{1z}] \neq 0$ $[J^2, J_{2z}] \neq 0$

es: $J_1^2 | j_1 j_2 ; j, m\rangle = j_2(j_2+1)\hbar^2 | j_1 j_2 ; j, m\rangle$

$|j_1 j_2 ; m_1 m_2\rangle = |m_1, m_2\rangle \quad |j_1 j_2 ; j, m\rangle = |j, m\rangle$

$$|J, m\rangle = \sum_{m_1 m_2} |m_1, m_2\rangle\langle m_1, m_2 | J, m\rangle$$

(linear combinations) CG coe.

Selection rule, $m = m_1 + m_2$

$|j_1 - j_2| \leq j \leq |j_1 + j_2|$

$$|\langle m_1, m_2 | j, m\rangle|^2 = 1 \quad \text{orthonormal condition}$$

CGe coe

$|0, 1\rangle = 1$

$|1, 0\rangle = \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}$

$|1, -1\rangle = 1$

$|0, 0\rangle = -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}$

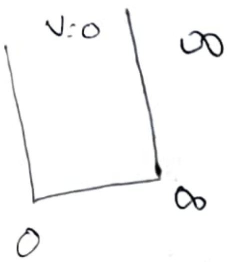
$$U = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & +\frac{1}{\sqrt{2}} & 0 \\ 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} |0\ 0\rangle \\ |0\ 0\rangle \\ |1\ 0\rangle \\ |1\ -1\rangle \end{bmatrix}$$

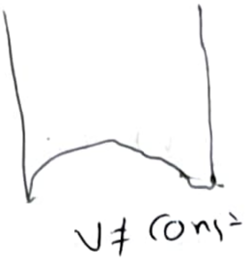
WKB Aproximation

Wentzel - Kramer - Brillowin method

This is the Aproximation for the System having slowly varing Potential.



Shrödinger



WKB method.

- Potential remain almost constant over a region of the order of De brogly wavelength.
- WKB method is vied as semi-classical Aproximation.
- In the case of classical System this property is always satisfied, since the wavelenth of the classical system ~ 0.

General Formulationism

Motion of particle in time indipendend potential

Shrodiger eqn = $-\frac{\hbar^2}{2m}\nabla^2\psi(r) + V(r)\psi = E\,\psi(r)$

$$\nabla^2\psi(r) + \frac{1}{\hbar^2}P^2(r)\,\psi(r) = 0 \quad -①$$

$P(r)$ is classical momentum at $\vec{r}$ => $P(r) = \sqrt{2m(E-V)}$

Particle moving in a region where potential is const. solution is given by

$$\psi(r) = Ae^{\pm i p \cdot r/\hbar}$$

$\psi = Ae^{\frac{i}{\hbar}E \ldots}$

If Potential is not const. (but const in debroglie wave length region)

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m(E-V)}}$$

WKB solution is given As

$$\psi(r) = A(r)e^{iS(r)/\hbar} \quad -②$$

, $A(r)$ = amplitude of WKB
S = phase factor

How to find $A(r)$ & $S(r)$

② in ① =>

Product rule

$\nabla^2\psi =$

$$\nabla^2\left(A(r)e^{iS(r)/\hbar}\right) \Rightarrow \nabla\left(e^{iS/\hbar}\nabla A + Ae^{iS/\hbar}\frac{i}{\hbar}\nabla S\right)$$

$$= Ae^{iS/\hbar}\frac{i}{\hbar}\nabla S + e^{iS/\hbar}\nabla^2 A + \frac{i}{\hbar}\nabla S\left(\nabla Ae^{iS/\hbar} + \frac{iA}{\hbar}\nabla S e^{iS/\hbar}\right)$$
$$+ Ae^{iS/\hbar} \cdot \frac{i}{\hbar}\nabla^2 S$$

$$= e^{iS/\hbar}\left[\frac{2Ai\nabla S}{\hbar}\right.$$

$$① \Rightarrow A\left[\frac{\hbar^2}{A}\nabla^2 A - (\nabla S)^2 + p^2\right] + i\hbar\left[(2\nabla A)\cdot(\nabla S) + A\nabla^2 S\right] = 0 \quad -③$$

Real & img. Part of Part of ③ must vanish seperately.

$\hbar^2 \rightarrow 0$ neglet

$$(\nabla S)^2 = p^2 = 2m(E-V) \quad -④$$

$$2(\nabla A)\cdot(\nabla S) + A\nabla^2 S = 0 \quad -⑤$$

④ & ⑤ in 1 D

$$\frac{dS}{dx} = \pm p(x) = \pm\sqrt{2m(E-V)} \quad -⑥$$

$$\frac{d^2}{dx^2}S \Rightarrow \frac{d}{dx}$$

$$2\left(\frac{d}{dx}A\right)P(x) + A\frac{d}{dx}P(x) = 0 \quad \div A$$

or

$$\frac{2}{A}\left(\frac{d}{dx}A\right)P(x) + \frac{d}{dx}P(x) = 0 \quad \div P(x)$$

$$\frac{d}{dx}\left[2\ln A + \ln P(x)\right] = 0$$

$$\int \left[\;\right] dx = \int 0\, dx$$

$$\ln A^2 + \ln P(x) = \ln c^2$$

$$\ln A^2 = \ln\left(\frac{c^2}{P(x)}\right)$$

$$A(x) \quad A = \frac{c}{\sqrt{|P(x)|}} \quad -⑧$$

From ⑥ $\Rightarrow$ $S(x)$

$$S = \pm\int P(x)\,dx = \pm\int dx\sqrt{2m(E-V)} \quad -⑦$$

Put S & A in ② $\Rightarrow$

$$\psi_{\pm}(x) = \frac{C_{\pm}}{\sqrt{|P(x)|}} \exp\left[\pm \frac{i}{\hbar} \int P(x')\, dx'\right]$$

Aproximate Solution of WKB

Amplitude (probability) $\propto \frac{1}{\sqrt{P(x)}}$

x is part of A

x' Part of S

Two cases: $E > V(x)$ ~ classicaly allowed region
$E < V(x)$ – classicaly forbidden region

Case I, $E > V(x)$

Solution is Oscilation nature

$$\psi(x) = \frac{C_+}{\sqrt{P(x)}} \exp\left[\frac{i}{\hbar} \int^{x} P(x')\, dx'\right] + \frac{C_-}{\sqrt{P(x)}} e\left[-\frac{i}{\hbar} \int^{x} P(x')\, dx'\right] \quad - (10)$$

$P(x) = \sqrt{2m(E-V)}$
$\Rightarrow$ +ve

Case II
$E < V(x)$

exponential decay

$$\psi(x) = \frac{C'_-}{\sqrt{|P(x)|}} \exp\left[-\frac{i}{\hbar} \int_{x} P(x')\, dx\right] + \frac{C'_+}{\sqrt{P(x)}} \exp\left[\frac{i}{\hbar} \int_{x} P(x')\, dx\right] \quad - (11)$$

$P(x) < 0$

Case

Case III $E = V \Rightarrow P(x) = 0$

$\psi(x) =$ The value of x at which momentum become '0', classical turning point

Particle stop & move to opposite direction

$\psi(x) \rightarrow \infty$ we can not solve in WKB

Validity of WKB Aproximation

By examing (size of terms in ③

$A(\nabla S)^2$ and $i\hbar A \nabla^2 S$ since $\hbar <<$

$|\hbar \nabla^2 S| << (\nabla S)^2$ — ①

In 1D => $\hbar \left| \frac{S''}{S'^2} \right| << 1$ — ② $S'' = \frac{d^2 S}{dx^2} = \nabla^2 S$

$S' = \frac{dS}{dx} = \nabla S$

② => $\left| \frac{d}{dx}\left(\frac{\hbar}{S'}\right) \right| << 1$

$S' = \frac{dS}{dx} = P(x)$; $\frac{d}{dx}\left(\frac{\hbar}{P(x)}\right) << 1$

$\left| \frac{d \bar{\lambda}(x)}{dx} \right| << 1$

$\lambda = \frac{h}{P}$; $\frac{\lambda}{2\pi} = \frac{h}{2\pi P}$

$\bar{\lambda} = \frac{\lambda}{2\pi}$

$\bar{\lambda} = \frac{\hbar}{P(x)} = \frac{\hbar}{\sqrt{2m(E-V)}}$ * de broglie wavelth

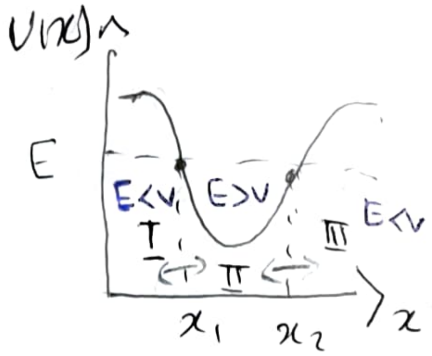
$$\left| \frac{d\bar{\lambda}}{dx} \right| = \left| \frac{d}{dx}\left(\frac{\hbar}{P}\right) \right| << 1$$

change in the 'λ' will be small

Finding Energy levels

Bound State for Potential wells with no rigid wall

E incident particle Energy



at x_1 & x_2 $E = V \Rightarrow P = 0$

classical turning point

$$P(x) = \pm\sqrt{2m(E-V)} = 0$$

$V - V$

$$\psi(x) \propto \frac{1}{\sqrt{P(x)}} \sim \infty$$

How to connect 3 region (10 & 11)

$$\psi_1 = \frac{c_1}{\sqrt{|P(x)|}} \exp\left[\frac{-1}{\hbar}\int_x^{x_1} P(x')\,dx'\right] + \left(\text{+ve term Diverge.}\right) \quad x < x_1$$

$$\psi_2 = \frac{c_2'}{\sqrt{P(x)}} \exp\left[\frac{i}{\hbar}\int_x P(x')\,dx'\right] + \frac{c_2''}{\sqrt{P(x)}} \exp\left[\frac{-i}{\hbar}\int_x P(x')\,dx'\right]$$

$$\psi_3 = \frac{c_3}{\sqrt{|P(x)|}} \exp\left[-\frac{1}{\hbar}\int_{x_2}^{x} P(x')\,dx\right] + \left[\text{+ve diverse}\right] \quad x > x_2$$

Connect ① to ② & ③ to ②

connection of ψ_3 to ψ_2

$$\psi_2 = \frac{C_2'}{\sqrt{p(x)}} \exp\left[\frac{i}{\hbar}\int_x^{x_2} p(x')\,dx'\right] + \frac{C_2''}{\sqrt{p(x)}} \exp\left[\frac{-i}{\hbar}\int_x^{x_2} p(x')\,dx'\right] \quad (4)$$

$$\psi_2 = \frac{C_2}{\sqrt{px}} \sin\left(\frac{1}{\hbar}\int_x^{x_2} p(x')\,dx + \alpha\right) \quad (5)$$

phase factor to determine

when we are going from (2) → (3) there will be a phase change.

Solve refer text $\Rightarrow \alpha = \frac{\pi}{4}$

$x_1 < x < x_2$

$$\psi_2 = \frac{C_2}{\sqrt{P(x)}} \sin\left(\frac{1}{\hbar}\int_x^{x_2} p(x')\,dx' + \frac{\pi}{4}\right)$$

similarly connect wavefn from ψ_1 to ψ_2

Phase factor again $\frac{\pi}{4}$

$$\psi_2 = \frac{D}{\sqrt{p(x)}} \sin\left[\frac{1}{\hbar}\int_{x_1}^{x} p(x')\,dx' + \beta\right] \quad — (6)$$

Next task to find out Energy

(5) & (6) ~~both~~ both are Solution of ψ_2 So they must be equal.

$$\Rightarrow \psi_2 = \frac{D}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int_{x_1}^{x} p(x')\,dx' + \frac{\pi}{4}\right) = \frac{C_2}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int_x^{x_2} p(x')\,dx' + \frac{\pi}{2}\right)$$

$$D \sin\theta_1 = C_2 \sin\theta_2$$

correct if if $(\theta_1 + \theta_2) = (n+1)\pi$ & $D = (-1)^n C_2$

$$\Rightarrow \left(\frac{1}{\hbar}\int_{x_1}^{x} P(x')\,dx' + \frac{\pi}{4}\right) + \left(\frac{1}{\hbar}\int_x^{x_2} p(x')\,d(x') + \frac{\pi}{4}\right) = (n+1)\pi$$

$$\boxed{\frac{1}{\hbar}\int_{x_1}^{x_2} p(x')\,dx' = \left(n+\frac{1}{2}\right)\pi}, \quad n = 0, 1, 2, \ldots$$

$\hbar = \frac{h}{2\pi}$

Particle move $x_1 \longrightarrow x_2$

$$\oint p(x)\,dx = 2\int_{x_1}^{x_2} p(x)\,dx = \left(n+\frac{1}{2}\right)h$$

full cycle

Sus

WKB energy levels are Quantized. & similar to that of Bohr Summerfield. Quantized f...

(8) ⇒ $\oint P(x,E) = 2\int_{x_1}^{x_2} \sqrt{2m(E_n - V(x))}\, dx = \left(n+\frac{1}{2}\right) h$

$\oint P(x)\, dx$ = Area Enclosed by the closed trajectory of particle in xp phase space.

Area between 2 successive boundstate =

$\oint P(x, E_{n+1})dx - \oint P(x, E_n)\, dx = \left[\left(n+\frac{1}{2}+1\right) - \left(n+\frac{1}{2}\right)\right]h$

$= h$

⇒ Each single state corresponds to the 'h' (area) in phase space.

<u>Example</u>

WKB to estimate Energy level of 1D harmonic oscillator

$E(x,p) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$

$P(x) = \pm\sqrt{2mE - m^2\omega^2 x^2}$

at turning points

$E = V(x) = \frac{1}{2} m\omega^2 x^2$

$x = \pm\sqrt{2E/m\omega^2}$

$x_{min} = -a$

$x_{max} = a$

$\oint p(x)\, dx = 2\int_{-a}^{a} \sqrt{2mE - m^2\omega^2 x^2}\, dx$

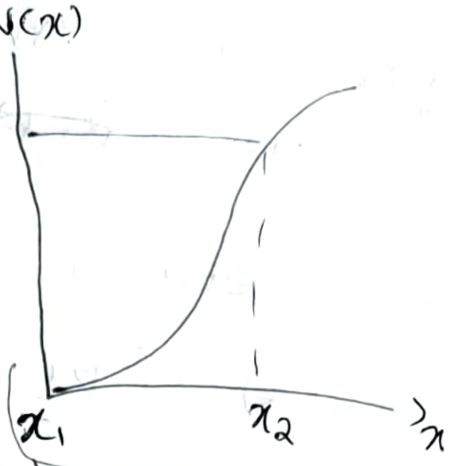
$= 2\times 2\int_0^a \left(\sqrt{2E/m\omega^2 - x^2}\right) m\omega\, dx$

$= 4m\omega \int_0^a \sqrt{a^2 - x^2}\, dx$

Put $x = a\sin\alpha$ ⇒ $= 4m\omega \int_0^{\pi/2} \left(\sqrt{1-\sin^2\alpha}\right) a^2\, d\alpha$ (cos α)

Boundstate for potential well with one rigid wall

$$\psi_{WKB} = \frac{A}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int p(x')\,dx' + \alpha\right)$$



$$x_1 \le x \le x_2$$

$$\psi_{WKB} = \frac{B}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int_{x}^{x_2} p(x')\,dx' + \pi/4\right) \quad -②$$

θ_1

wavefunction will vanish at rigid wall ie $x = x_1$

So $\psi_{WKB} = \frac{A}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int_{x_1}^{x} p(x')\,dx' + 0\right)$ ③

θ_2

Since ② = ③

$\Rightarrow \theta_1 + \theta_2 = (n+1)\pi$, $A = (-1)^n B$

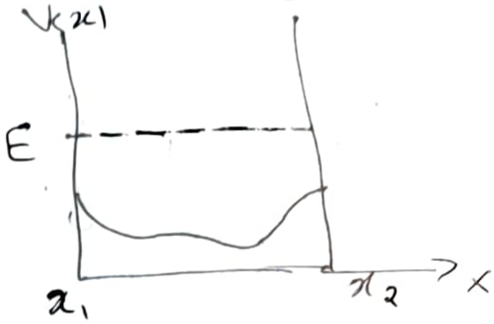
$$\frac{1}{\hbar}\int_{x_1}^{x} p(x')\,dx' + \frac{1}{\hbar}\int_{x}^{x_2} p(x')\,dx' + \pi/4 = (n+1)\pi \quad -④$$

$$\Rightarrow \int_{x_1}^{x_2} p(x)\,dx = \left(n + \frac{3}{4}\right)\pi\hbar \quad , n = 0, 1, 2, 3, \ldots$$

Quntization rule.

Boundstate for potential well with two rigid walls

$$\psi_{WKB} = \frac{A}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int_{x_1}^{x} p(x')\,dx'\right) \quad (x > x_1)$$



$x_1 < x < x_2$

$(x < x_2)$

$$\psi_{WKB} = \frac{B}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int_{x}^{x_2} p(x')\,dx'\right) \quad x_1 < x < x_2$$

$\theta_1 + \theta_2 = (n+1)\pi \qquad A = (-1)^n B$

$$\frac{1}{\hbar}\int_{x_1}^{x} p(x')\,dx' + \frac{1}{\hbar}\int_{x}^{x_2} p(x')\,dx' = (n+1)\pi$$

$$\int_{x_1}^{x} p(x')\,dx = (n+1)\pi \quad , n = 0, 1, 2, \ldots$$

$$\boxed{\int_{x_1}^{x_2} p(x)\,dx' = n\pi\hbar \quad n = 1, 2, 3, \ldots}$$

Problem: Use the WKB approximation to calculate the energy levels of spinless particle of mass m moving in one dimensional box with walls at $x = 0$ $x = L$

$$\int_{x_1}^{x_2} p(x)\,d(x') = n\pi\hbar$$

$$P(E, x) = \sqrt{2mE},$$

$$\int_0^L p(x)\,dx = \int_0^L \sqrt{2mE}\,dx = n\pi\hbar$$

$$\sqrt{2mE_n^{WKB}} \times L = n\pi\hbar$$

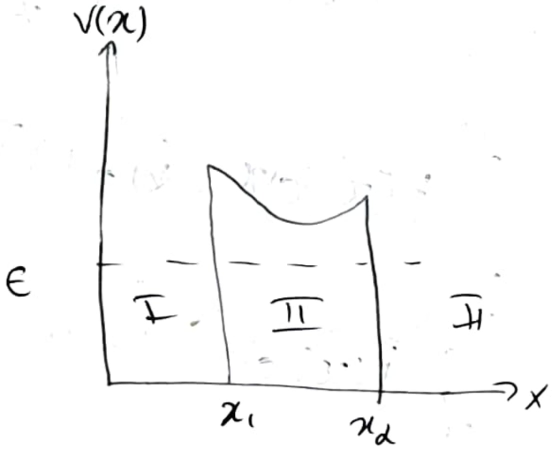
$$\boxed{E_n^{WKB} = \frac{\pi^2\hbar^2}{2mL^2} n^2}$$

Tunnuling through the potential barrier

$$\psi_1 = Ae^{ip_0x/\hbar} + Be^{-ip_0x/\hbar} \quad ①$$

$$\psi_3 = Ee^{ip_0x/\hbar} \quad ②$$

$$, \; p_0 = \sqrt{2mE}$$



$$\psi_2(x) = \frac{c}{\sqrt{|p(x)|}} \exp\left[-\frac{1}{\hbar}\int_{x_1}^{x_2} |p(x')|\,dx'\right] +$$

$$p(x) = i\sqrt{2m(V-E)}$$

Transmission coe.

v = speed

$$T = \frac{v_{tra}}{v_{inc}} \frac{|\psi_{tra}(x)|^2}{|\psi_{inc}(x)|^2} = \frac{|E|^2}{|A^2|}$$

Boundary Condition

$$\psi_1(x_1) = \psi_2(x_1)$$

$$\frac{d}{dx}\psi_1(x_1) = \frac{d}{dx}\psi_2(x_1)$$

$$\psi_2(x_2) = \psi_3(x_2)$$

$$\frac{d}{dx}\psi_2(x_3) = \frac{d}{dx}\psi_3(x_2)$$

$$\frac{E}{A} = \frac{2}{1 - a_1/ip_0}\sqrt{\frac{a_1}{a_2}}\, e^{ip_0(x_1 - x_2)/\hbar}$$

$$\frac{|E|^2}{|A|^2} = \frac{4}{\frac{a_2}{a_1} + \frac{a_1 a_2}{p_0^2}} \exp\left[\frac{-2}{\hbar}\int_{x_1}^{x_2} |p(x)|\, dx\right]$$

$$T \sim e^{-2\gamma}, \quad \gamma = \frac{1}{\hbar}\int_{x_1}^{x_2} \sqrt{2m(V(x) - E)}\, dx$$

Tunneling also occurs with metals, when metal is subjected to extreme electric field. thus e- can be emmited from the metal this is known as cold emmision of electron

exap: Use WKB aproximation to estimate the transmission coe of of particle of mass m and Energy E moving in the following potential barrier.

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 - \lambda . x & x > 0 \end{cases}$$

$$T = e^{-\gamma} \qquad \gamma = \frac{1}{\hbar} \int_{x_1}^{x_2} \sqrt{2m(V(x) - E)}\, dx$$

$x_1 = 0$, $x_2 \Rightarrow V_0 - \lambda x_2 = E$

$$x_2 = \frac{V_0 - E}{\lambda}$$

$$V - E = V_0 - E - \lambda x$$

$$\gamma = \frac{1}{\hbar} \int_{x_1}^{x_2} \sqrt{2m(V-E)}\, dx = \int_{x_1=0}^{x_2 = \frac{V_0 - E}{\lambda}} \sqrt{2m(V_0 - E - \lambda x)}\, dx$$

$$= \frac{\sqrt{2m}}{\hbar} \int_0^{\frac{V_0 - E}{\lambda}} \sqrt{V_0 - E - \lambda x}\, dx$$

~~$V_0 - E - \lambda x = P$~~

~~$-\lambda\, dx = dP$~~

~~$dx = \frac{-dP}{\lambda}$~~

$$\gamma = \frac{\sqrt{2m}}{\hbar} \int \frac{1}{\lambda} \sqrt{p}\, dp$$

$$\gamma = \frac{\sqrt{2m}}{\hbar} \left[\frac{2 (V_0 - E - \lambda x)^{3/2}}{-3\lambda} \right]_0^{\frac{V_0 - E}{\lambda}}$$

$$= \frac{2\sqrt{2m}}{+3\hbar\lambda} \left[(V_0 - E)^{3/2} - V_0 - E - x \left(\frac{V_0 - E}{\lambda} \right) \right.$$

$$\gamma = \frac{2\sqrt{2m}}{3\hbar\lambda} (V_0 - E)^{3/2}$$

$$T \sim e^{-2\gamma} = \exp\left\{ -\frac{4\sqrt{2m}}{3\hbar\lambda} (V_0 - E)^{3/2} \right\}$$

$\varepsilon =$ electric fiad

$$V = V_0 - e^{\varepsilon \cdot x}$$

$\lambda = e\varepsilon \Leftarrow$ cold emmision

WKB aproximation

$$\nabla^2\psi(r) + \frac{P(r)}{\hbar^2}\psi(r) = 0 \quad , \quad P(r) = \sqrt{2m(E - V(r))}$$

$A(r)$ = amplitud

$S(r)$ = phase factor.

$$\psi(\vec{r}) = A(\vec{r})\, e^{iS(\vec{r})/\hbar}$$

$$\Rightarrow \frac{dS}{dx} = \pm p(x) \Rightarrow S = \int p(x)\,dx$$

$$A = \frac{C}{\sqrt{|p(x)|}}$$

$$\psi_\pm(x) = \frac{C_\pm}{\sqrt{|p(x)|}} \exp\left[\pm\frac{i}{\hbar}\int^x p(x')\,dx'\right]$$

$E > V(x)$ (case I)

$E < V(x)$ case II ($i \times i = -1$)

GS $\Rightarrow \psi_+ + \psi_-$

No rigid walls

$$\oint p(x)\,dx = \left(n+\frac{1}{2}\right)h \Rightarrow \int_{x_1}^{x_2} p(x)\,dx = \left(n+\frac{1}{2}\right)\pi\hbar$$

$$D\sin\theta_1 = C_2\sin\theta_2 \Rightarrow \theta_1 + \theta_2 = (n+1)\pi$$

$$D = (-1)^n C_2$$

One rigid wall

$$\int_{x_1}^{x_2} p(x)\,dx = \left(n+\frac{3}{4}\right)\pi\hbar$$

Two rigid walls

$$\int_{x_1}^{x_2} p(x)\,dx = (n+1)\pi\hbar, \quad n = 0, 1, 2, \ldots$$

$$= n\pi\hbar \quad n = 1, 2, \ldots$$

phase factor '0' for rigid walls, $\pi/4$ for non rigid

Tunnelling

$$T = \frac{v_{tra}\,|\psi_{tra}(x)|^2}{v_{inc}\,|\psi_{in}(x)|^2} = \frac{|E|^2}{|A|^2}$$

$p(x) = \sqrt{V(x) - E}$

otherwise (i)

$$T \simeq e^{-2\gamma l}, \quad \gamma l = \frac{1}{\hbar}\int_{x_1}^{x_2} p(x)\,dx$$

Harmonic oscillator

$$\psi_n(x) = \frac{1}{\sqrt{\sqrt{\pi}\,2^n n!}}\,\frac{1}{x_0^{n+1/2}}\left(x - x_0^2\frac{d}{dx}\right)^n e^{-x^2/2x_0^2}$$

L	T	P	Cr
4	0	0	4

Course Code: PHY.508
Course Title: Quantum Mechanics
Total Hours: 60

Learning Outcomes: Learning Outcomes:
At the end of course students will able to:

- Explain mathematical formulation of quantum mechanics.
- Apply Schrodinger's equation to solve eigen value problems such as box potential, harmonic oscillator, hydrogen atom and quantum mechanical tunneling.
- Formulate C G coefficients using angular momentum algebra.
- Outline WKB method and bound states of potentials well.
- Explain scattering theory for various kind of potential problems.

Course Contents

Unit-I **14 hours**

Mathematical Formulation and Postulates of Quantum Mechanics: Limitations of Classical Mechanics and foundation of Quantum Mechanics, Review of linear vector spaces and related algebra and Hilbert space, Dirac notation, Operators: Hermitian, Unitary & Projection operators, Matrix representations of kets, bras and operators, Change of basis, Basic postulates of quantum mechanics, Schrödinger wave equation (time dependent and time independent), Expectation values, Commutation relations, Ehrenfest theorem. Generalized Heisenberg uncertainty principle, density matrix, Schrodinger, Heisenberg and Interaction pictures.

Unit-II **16 hours**

Applications of Schrödinger Wave Equation: Solution of Harmonic oscillator using wave mechanics and matrix mechanics: matrix representation and eigen values of various operators, Anisotropic and isotropic harmonic oscillator, The box potential.
Hydrogen Atom: Motion in central potential, Solution of Schrodinger equation for hydrogen atom. energy spectra of Hydrogen atom.
Angular Momentum: eigenvalues and eigen vectors of orbital angular momentum, Spherical harmonics, Angular momentum algebra and commutation relations, Matrix representation of angular momentum, Stern-

Gerlach experiment, Spin angular momentum: Pauli matrices and their properties.

Unit-III **16 hours**

Addition of Angular Momenta: Addition of two angular momenta, Transformation between bases: Clebsch-Gordan Coefficients, Eigenvalues of J^2 and J_z, Coupling of orbital and spin angular momenta. Wigner-Eckart Theorem (statement only)
WKB Method and its Applications: General formulation of WKB method, validity of WKB approximation, Bound states of potential wells with zero, one and two rigid walls, Application of WKB method to barrier penetration and cold emission of electrons from metals.

Unit-IV **14 hours**

Scattering Theory: Quantum Scattering theory, Scattering cross-section and scattering amplitude, Born scattering formula, Central force problem, Partial wave analysis, Phase shifts, Optical theorem, Low energy s-wave and p-wave scatterings, Bound states and resonances, Breit-Wigner resonance formula (statement only), Green's functions in scattering theory, Born approximation and its validity, Scattering for different kinds of potentials, Scattering of identical particles.

Transaction Mode:
Lecture, demonstration, tutorial, problem solving.

Suggested Readings:

1. Zettili N.(2009). *Quantum Mechanics-Concepts and Applications.* Sussex, U.K: John Wiley & Sons Ltd.
2. Merzbacher E.(2011). *Quantum Mechanics.* New Delhi, India: Wiley India Pvt. Ltd.
3. Schiff L.I.(2010). *Quantum Mechanics* . Noida, India: McGraw-Hill Education.
4. Venkatesan K and Mathews,P.M.(2010). *A Textbook of Quantum Mechanics.* Noida, India: Tata McGraw - Hill Education.
5. Sakurai J. J.(2009). *Modern Quantum Mechanics.* India: Pearson Education.
6. Griffiths D. J.(2015). *Introduction to Quantum Mechanics*, India: Pearson Education.
7. Mahan G. D.(2009). Quantum Mechanics in a Nutshell. Princeton University Press.